Figure 1

Table 1. Crystallographic data and refinement statistics

	Native data set
Wavelength (Å)	1.0526
Resolution range (Å)[1]	50.0-2.0 (2.07-2.0)
No. of observed reflections	164,206
No. of unique reflections	27,881
No. of reflections in R_{free} set	828
Completeness (%)	99.2(99.4)
I/σ(I)	19.6(1.4)
(R_{merge}) (%)[2]	3.9(20.9)
R_{cryst}/R_{free} (%)[3]	21.8/23.8
No. of refined non-hydrogen atoms[4]	
protein	2248
water	265
Average B-factor (all atoms, Å^2)	60
Wilson B-factor (Å^2)	45
R.m.s. Δ bond lengths/angles[5]	0.0081/1.7
Residues in allowed regions (%)[6]	97%

[1]Values in parentheses are statistics for the highest resolution bin.
[2]$R_{merge}\ (I) = \sum_{hkl} |Ihkl - < Ihkl >| / \sum_{hkl} Ihkl$, where $Ihkl$ is the measured intensity of the reflections with indices *hkl*.
[3]$R = \sum_{hkl} \| Fo| - |Fc\| / \sum |Fo|$, where $|Fo|$ and $|Fc|$ are the observed and calculated structure factor amplitudes for reflection hkl, applied to the work (R_{cryst}=97%) and test (R_{free}=3%) sets, respectively.
[4]Residues -2, 239 and 240 were not located. Residues originating from the cloning site were given negative integers.
[5]Root mean squared deviations (rms Δ) in bond length and angles from ideal values.
[6]The Ramachandran plot was calculated according to Kleywegt and Jones, (1996).

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Figure 2 (Table 2 (page 1))

```
HEADER    CELL ADHESION                                1QZ1
TITLE     CRYSTAL STRUCTURE OF THE IG 1-2-3 FRAGMENT OF NCAM
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: NEURAL CELL ADHESION MOLECULE 1, 140 KDA ISOFORM;
COMPND   3 CHAIN: A;
COMPND   4 FRAGMENT: IG MODULES 1-2-3;
COMPND   5 SYNONYM: N-CAM 140, NCAM-140;
COMPND   6 ENGINEERED: YES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: RATTUS NORVEGICUS;
SOURCE   3 ORGANISM_COMMON: RAT;
SOURCE   4 GENE: NCAM1;
SOURCE   5 EXPRESSION_SYSTEM: PICHIA PASTORIS;
SOURCE   6 EXPRESSION_SYSTEM_COMMON: FUNGUS;
SOURCE   7 EXPRESSION_SYSTEM_STRAIN: GS-115;
SOURCE   8 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE   9 EXPRESSION_SYSTEM_PLASMID: PHIL-S1
KEYWDS    IG MODULES, CELL ADHESION, NCAM
EXPDTA    X-RAY DIFFRACTION
AUTHOR    V.SOROKA, K.KOLKOVA, J.S.KASTRUP, K.DIEDERICHS, J.BREED,
AUTHOR   2 V.V.KISELYOV, F.M.POULSEN, I.LARSEN, W.WELTE, V.BEREZIN,
AUTHOR   3 E.BOCK, C.KASPER
JRNL        AUTH   V.SOROKA, K.KOLKOVA, J.S.KASTRUP, K.DIEDERICHS,
JRNL        AUTH 2 J.BREED, V.V. KISELYOV, F.M.POULSEN, I.LARSEN,
JRNL        AUTH 3 W.WELTE, V.BEREZIN, E.BOCK, C.KASPER
JRNL       TITL   STRUCTURE AND INTERACTIONS OF NCAM IG1-2-3 SUGGEST
JRNL       TITL 2 A NOVEL ZIPPER MECHANISM FOR HOMOPHILIC ADHESION
JRNL        REF    TO BE PUBLISHED
JRNL        REFN
REMARK   1
REMARK   1 REFERENCE 1
REMARK   1  AUTH   C.KASPER,H.RASMUSSEN,J.S.KASTRUP,S.IKEMIZU,
REMARK   1  AUTH 2 E.Y.JONES,V.BEREZIN,E.BOCK,I.K.LARSEN
REMARK   1  TITL   STRUCTURAL BASIS OF CELL-CELL ADHESION BY NCAM
REMARK   1  REF    NAT.STRUCT.BIOL.              V.   7   389 2000
REMARK   1  REFN   ASTM NSBIEW  US ISSN 1072-8368
REMARK   1 REFERENCE 2
REMARK   1  AUTH   C.KASPER,H.RASMUSSEN,V.BEREZIN,E.BOCK,I.K.LARSEN
REMARK   1  TITL   EXPRESSION, CRYSTALLIZATION AND PRELIMINARY X-RAY
REMARK   1  TITL 2 ANALYSIS OF THE TWO AMINO-TERMINAL IG DOMAINS OF
REMARK   1  TITL 3 THE NEURAL CELL ADHESION MOLECULE (NCAM)
REMARK   1  REF    ACTA CRYSTALLOGR., SECT.D     V.  55  1598 1999
REMARK   1  REFN   ASTM ABCRE6  DK ISSN 0907-4449
REMARK   2
REMARK   2 RESOLUTION. 2.00 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM      : CNS 1.0
REMARK   3   AUTHORS      : BRUNGER,ADAMS,CLORE,DELANO,GROS,GROSSE-
REMARK   3                : KUNSTLEVE,JIANG,KUSZEWSKI,NILGES, PANNU,
REMARK   3                : READ,RICE,SIMONSON,WARREN
REMARK   3
REMARK   3  REFINEMENT TARGET : ENGH & HUBER
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 2.00
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 48.64
```

Figure 2 (Table 2 (page 2))

```
REMARK   3   DATA CUTOFF            (SIGMA(F)) : 0.000
REMARK   3   DATA CUTOFF HIGH          (ABS(F)) : NULL
REMARK   3   DATA CUTOFF LOW           (ABS(F)) : NULL
REMARK   3   COMPLETENESS (WORKING+TEST)    (%) : 99.2
REMARK   3   NUMBER OF REFLECTIONS              : 28289
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD            : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION    : RANDOM
REMARK   3   R VALUE             (WORKING SET) : 0.218
REMARK   3   FREE R VALUE                       : 0.238
REMARK   3   FREE R VALUE TEST SET SIZE   (%)   : NULL
REMARK   3   FREE R VALUE TEST SET COUNT        : 828
REMARK   3   ESTIMATED ERROR OF FREE R VALUE    : NULL
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED             : NULL
REMARK   3   BIN RESOLUTION RANGE HIGH       (A)  : 2.00
REMARK   3   BIN RESOLUTION RANGE LOW        (A)  : 2.13
REMARK   3   BIN COMPLETENESS (WORKING+TEST) (%)  : 99.00
REMARK   3   REFLECTIONS IN BIN    (WORKING SET)  : NULL
REMARK   3   BIN R VALUE           (WORKING SET)  : 0.3730
REMARK   3   BIN FREE R VALUE                     : 0.4390
REMARK   3   BIN FREE R VALUE TEST SET SIZE  (%)  : NULL
REMARK   3   BIN FREE R VALUE TEST SET COUNT      : 148
REMARK   3   ESTIMATED ERROR OF BIN FREE R VALUE  : 0.036
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 2247
REMARK   3   NUCLEIC ACID ATOMS       : 0
REMARK   3   HETEROGEN ATOMS          : 0
REMARK   3   SOLVENT ATOMS            : 265
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : 42.00
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : 60.60
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) : 7.90000
REMARK   3    B22 (A**2) : -15.20000
REMARK   3    B33 (A**2) : 7.30000
REMARK   3    B12 (A**2) : 0.00000
REMARK   3    B13 (A**2) : 0.00000
REMARK   3    B23 (A**2) : 0.00000
REMARK   3
REMARK   3  ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM LUZZATI PLOT        (A) : 0.30
REMARK   3   ESD FROM SIGMAA              (A) : 0.36
REMARK   3   LOW RESOLUTION CUTOFF        (A) : 5.00
REMARK   3
REMARK   3  CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM C-V LUZZATI PLOT    (A) : 0.35
REMARK   3   ESD FROM C-V SIGMAA          (A) : 0.42
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   BOND LENGTHS                 (A) : 0.008
REMARK   3   BOND ANGLES            (DEGREES) : 1.70
REMARK   3   DIHEDRAL ANGLES        (DEGREES) : 27.50
```

Figure 2 (Table 2 (page 3))

```
REMARK   3   IMPROPER ANGLES        (DEGREES) : 0.95
REMARK   3
REMARK   3  ISOTROPIC THERMAL MODEL : ANISOTROPIC
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.     RMS     SIGMA
REMARK   3   MAIN-CHAIN BOND              (A**2) : NULL  ; NULL
REMARK   3   MAIN-CHAIN ANGLE             (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN BOND              (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN ANGLE             (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  BULK SOLVENT MODELING.
REMARK   3   METHOD USED : NULL
REMARK   3   KSOL        : NULL
REMARK   3   BSOL        : NULL
REMARK   3
REMARK   3  NCS MODEL : NULL
REMARK   3
REMARK   3  NCS RESTRAINTS.                         RMS   SIGMA/WEIGHT
REMARK   3   GROUP  1  POSITIONAL            (A) : NULL  ; NULL
REMARK   3   GROUP  1  B-FACTOR           (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  PARAMETER FILE  1   : NULL
REMARK   3  TOPOLOGY FILE  1    : NULL
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: RESIDUES 241-242 WERE NOT LOCATED IN
REMARK   3  THE ELECTRON DENSITY MAP
REMARK   4
REMARK   4 1QZ1 COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 17-SEP-2003.
REMARK 100 THE RCSB ID CODE IS RCSB020242.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : 06-NOV-2000; 04-DEC-2000
REMARK 200  TEMPERATURE           (KELVIN) : 100.0
REMARK 200  PH                             : 5.20
REMARK 200  NUMBER OF CRYSTALS USED        : 1
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : Y; N
REMARK 200  RADIATION SOURCE               : MAX II ; ROTATING ANODE
REMARK 200  BEAMLINE                       : I711
REMARK 200  X-RAY GENERATOR MODEL          : NULL; HOME SOURCE
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : M
REMARK 200  WAVELENGTH OR RANGE        (A) : 1.0526; 1.54
REMARK 200  MONOCHROMATOR                  : NULL
REMARK 200  OPTICS                         : NULL
REMARK 200
REMARK 200  DETECTOR TYPE                  : IMAGE PLATE; IMAGE PLATE
REMARK 200  DETECTOR MANUFACTURER          : MARRESEARCH; MARRESEARCH
REMARK 200  INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200  DATA SCALING SOFTWARE          : SCALEPACK
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 27881
REMARK 200  RESOLUTION RANGE HIGH      (A) : 2.000
REMARK 200  RESOLUTION RANGE LOW       (A) : 50.000
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : 0.000
```

Figure 2 (Table 2 (page 4))

```
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%) : 99.2
REMARK 200  DATA REDUNDANCY                : 5.900
REMARK 200  R MERGE                    (I) : 0.03900
REMARK 200  R SYM                      (I) : 0.03900
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET  : 19.6000
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.00
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.07
REMARK 200  COMPLETENESS FOR SHELL     (%) : 99.4
REMARK 200  DATA REDUNDANCY IN SHELL       : 3.80
REMARK 200  R MERGE FOR SHELL          (I) : 0.20900
REMARK 200  R SYM FOR SHELL            (I) : 0.20900
REMARK 200  <I/SIGMA(I)> FOR SHELL         : 1.400
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
REMARK 200 SOFTWARE USED: AMORE
REMARK 200 STARTING MODEL: PDB ENTRY 1EPF
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): NULL
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 14-17% PEG 4000, 450 MM LI SULFATE,
REMARK 280  100 MM NA ACETATE, PH 5.2, VAPOR DIFFUSION, HANGING DROP,
REMARK 280  TEMPERATURE 293K
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: I 21 21 21
REMARK 290
REMARK 290      SYMOP   SYMMETRY
REMARK 290     NNNMMM   OPERATOR
REMARK 290       1555   X,Y,Z
REMARK 290       2555   1/2-X,-Y,1/2+Z
REMARK 290       3555   -X,1/2+Y,1/2-Z
REMARK 290       4555   1/2+X,1/2-Y,-Z
REMARK 290       5555   1/2+X,1/2+Y,1/2+Z
REMARK 290       6555   -X,1/2-Y,Z
REMARK 290       7555   1/2-X,Y,-Z
REMARK 290       8555   X,-Y,1/2-Z
REMARK 290
REMARK 290     WHERE NNN -> OPERATOR NUMBER
REMARK 290           MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290   SMTRY1   1  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   2 -1.000000  0.000000  0.000000       25.72000
```

Figure 2 (Table 2 (page 5))

```
REMARK 290   SMTRY2   2  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   2  0.000000  0.000000  1.000000       74.65000
REMARK 290   SMTRY1   3 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   3  0.000000  1.000000  0.000000       53.88000
REMARK 290   SMTRY3   3  0.000000  0.000000 -1.000000       74.65000
REMARK 290   SMTRY1   4  1.000000  0.000000  0.000000       25.72000
REMARK 290   SMTRY2   4  0.000000 -1.000000  0.000000       53.88000
REMARK 290   SMTRY3   4  0.000000  0.000000 -1.000000        0.00000
REMARK 290   SMTRY1   5  1.000000  0.000000  0.000000       25.72000
REMARK 290   SMTRY2   5  0.000000  1.000000  0.000000       53.88000
REMARK 290   SMTRY3   5  0.000000  0.000000  1.000000       74.65000
REMARK 290   SMTRY1   6 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   6  0.000000 -1.000000  0.000000       53.88000
REMARK 290   SMTRY3   6  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   7 -1.000000  0.000000  0.000000       25.72000
REMARK 290   SMTRY2   7  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   7  0.000000  0.000000 -1.000000        0.00000
REMARK 290   SMTRY1   8  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   8  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   8  0.000000  0.000000 -1.000000       74.65000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF 1 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000        0.00000
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465   M RES C SSSEQI
REMARK 465     ARG A    -2
REMARK 465     GLU A   239
REMARK 465     GLU A   240
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
```

Figure 2 (Table 2(page 6))

```
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATM1   ATM2   ATM3
REMARK 500   LEU A   1    N    -  CA   -  C    ANGL. DEV. = 11.0 DEGREES
REMARK 500   ASP A  27    N    -  CA   -  C    ANGL. DEV. = 11.4 DEGREES
REMARK 500   ALA A  28    N    -  CA   -  C    ANGL. DEV. =-17.5 DEGREES
REMARK 500   LYS A  29    N    -  CA   -  C    ANGL. DEV. = 12.7 DEGREES
REMARK 500   ASP A  56    N    -  CA   -  C    ANGL. DEV. =-11.4 DEGREES
REMARK 500   ALA A  89    N    -  CA   -  C    ANGL. DEV. =-10.5 DEGREES
REMARK 500   GLN A 108    N    -  CA   -  C    ANGL. DEV. =-10.5 DEGREES
REMARK 500   THR A 129    N    -  CA   -  C    ANGL. DEV. =-11.4 DEGREES
REMARK 500   ASP A 138    N    -  CA   -  C    ANGL. DEV. =-11.4 DEGREES
REMARK 500   ASP A 144    N    -  CA   -  C    ANGL. DEV. =-20.1 DEGREES
REMARK 500   THR A 194    N    -  CA   -  C    ANGL. DEV. =-11.0 DEGREES
REMARK 500   ARG A 257    N    -  CA   -  C    ANGL. DEV. = 17.3 DEGREES
REMARK 525
REMARK 525 SOLVENT
REMARK 525 THE FOLLOWING SOLVENT MOLECULES LIE FARTHER THAN EXPECTED
REMARK 525 FROM THE PROTEIN OR NUCLEIC ACID MOLECULE AND MAY BE
REMARK 525 ASSOCIATED WITH A SYMMETRY RELATED MOLECULE (M=MODEL
REMARK 525 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 525 NUMBER; I=INSERTION CODE):
REMARK 525
REMARK 525  M RES CSSEQI
REMARK 525    HOH    64        DISTANCE =  5.56 ANGSTROMS
REMARK 525    HOH    66        DISTANCE =  7.20 ANGSTROMS
REMARK 525    HOH    75        DISTANCE = 10.03 ANGSTROMS
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 2NCM   RELATED DB: PDB
REMARK 900 NMR STRUCTURE OF THE FIRST IMMUNOGLOBULIN DOMAIN OF THE
REMARK 900 NEURAL CELL ADHESION MOLECULE (NCAM)
REMARK 900 RELATED ID: 3NCM   RELATED DB: PDB
REMARK 900 NMR STRUCTURE OF THE SECOND IMMUNOGLOBULIN DOMAIN OF THE
REMARK 900 NEURAL CELL ADHESION MOLECULE (NCAM)
REMARK 900 RELATED ID: 1EPF   RELATED DB: PDB
REMARK 900 CRYSTAL STRUCTURE OF THE TWO N-TERMINAL IMMUNOGLOBULIN
REMARK 900 DOMAINS OF THE NEURAL CELL ADHESION MOLECULE (NCAM)
REMARK 999
REMARK 999 SEQUENCE
REMARK 999 RESIDUES -2, 239 AND 240 WERE NOT VISIBLE IN
REMARK 999 THE ELECTRON DENSITY.
DBREF  1QZ1 A    1   289  SWS    P13596   NCA1_RAT        20    308
SEQADV 1QZ1 ARG A   -2  SWS  P13596              CLONING ARTIFACT
SEQADV 1QZ1 VAL A   -1  SWS  P13596              CLONING ARTIFACT
SEQRES 1  A 291  ARG VAL LEU GLN VAL ASP ILE VAL PRO SER GLN GLY GLU
SEQRES 2  A 291  ILE SER VAL GLY GLU SER LYS PHE PHE LEU CYS GLN VAL
SEQRES 3  A 291  ALA GLY ASP ALA LYS ASP LYS ASP ILE SER TRP PHE SER
SEQRES 4  A 291  PRO ASN GLY GLU LYS LEU SER PRO ASN GLN GLN ARG ILE
SEQRES 5  A 291  SER VAL VAL TRP ASN ASP ASP SER SER THR LEU THR
SEQRES 6  A 291  ILE TYR ASN ALA ASN ILE ASP ASP ALA GLY ILE TYR LYS
SEQRES 7  A 291  CYS VAL VAL THR ALA GLU ASP GLY THR GLN SER GLU ALA
```

Figure 2 (Table 2 (page 7))

```
SEQRES 8  A 291  THR VAL ASN VAL LYS ILE PHE GLN LYS LEU MET PHE LYS
SEQRES 9  A 291  ASN ALA PRO THR PRO GLN GLU PHE LYS GLU GLY GLU ASP
SEQRES 10 A 291  ALA VAL ILE VAL CYS ASP VAL VAL SER SER LEU PRO PRO
SEQRES 11 A 291  THR ILE ILE TRP LYS HIS LYS GLY ARG ASP VAL ILE LEU
SEQRES 12 A 291  LYS LYS ASP VAL ARG PHE ILE VAL LEU SER ASN ASN TYR
SEQRES 13 A 291  LEU GLN ILE ARG GLY ILE LYS LYS THR ASP GLU GLY THR
SEQRES 14 A 291  TYR ARG CYS GLU GLY ARG ILE LEU ALA ARG GLY GLU ILE
SEQRES 15 A 291  ASN PHE LYS ASP ILE GLN VAL ILE VAL ASN VAL PRO PRO
SEQRES 16 A 291  THR VAL GLN ALA ARG GLN SER ILE VAL ASN ALA THR ALA
SEQRES 17 A 291  ASN LEU GLY GLN SER VAL THR LEU VAL CYS ASP ALA ASP
SEQRES 18 A 291  GLY PHE PRO GLU PRO THR MET SER TRP THR LYS ASP GLY
SEQRES 19 A 291  GLU PRO ILE GLU ASN GLU GLU GLU ASP ASP GLU LYS HIS
SEQRES 20 A 291  ILE PHE SER ASP ASP SER SER GLU LEU THR ILE ARG ASN
SEQRES 21 A 291  VAL ASP LYS ASN ASP GLU ALA GLU TYR VAL CYS ILE ALA
SEQRES 22 A 291  GLU ASN LYS ALA GLY GLU GLN ASP ALA SER ILE HIS LEU
SEQRES 23 A 291  LYS VAL PHE ALA LYS
FORMUL   2  HOH    *265(H2 O1)
HELIX    1   1 ASN A   68  ALA A   72  5                                    5
HELIX    2   2 LYS A  161  GLU A  165  5                                    5
HELIX    3   3 ASP A  260  GLU A  264  5                                    5
SHEET    1   A 4 VAL A   3  VAL A   6  0
SHEET    2   A 4 LYS A  18  VAL A  24 -1  O  GLN A  23   N  ASP A   4
SHEET    3   A 4 SER A  59  ILE A  64 -1  O  ILE A  64   N  LYS A  18
SHEET    4   A 4 ILE A  50  ASP A  56 -1  N  VAL A  53   O  THR A  61
SHEET    1   B 4 GLY A  10  SER A  13  0
SHEET    2   B 4 GLN A  86  PHE A  96  1  O  LYS A  94   N  GLY A   0
SHEET    3   B 4 GLY A  73  THR A  80 -1  N  VAL A  79   O  SER A  87
SHEET    4   B 4 ASP A  32  PHE A  36 -1  N  SER A  34   O  VAL A  78
SHEET    1   C 2 MET A 100  ASN A 103  0
SHEET    2   C 2 ASP A 121  VAL A 123 -1  O  ASP A 121   N  ASN A 103
SHEET    1   D 4 GLN A 108  LYS A 111  0
SHEET    2   D 4 GLU A 179  ALA A 197  1  O  ASN A 190   N  PHE A 110
SHEET    3   D 4 GLY A 166  ILE A 174 -1  N  GLY A 166   O  VAL A 187
SHEET    4   D 4 THR A 129  HIS A 134 -1  N  LYS A 133   O  ARG A 169
SHEET    1   E 5 GLN A 108  LYS A 111  0
SHEET    2   E 5 GLU A 179  ALA A 197  1  O  ASN A 190   N  PHE A 110
SHEET    3   E 5 VAL A 212  PHE A 221 -1  O  ASP A 217   N  GLN A 196
SHEET    4   E 5 GLU A 253  ILE A 256 -1  O  LEU A 254   N  LEU A 214
SHEET    5   E 5 HIS A 245  PHE A 247 -1  N  ILE A 246   O  THR A 255
SHEET    1   F 3 ALA A 116  ILE A 118  0
SHEET    2   F 3 LEU A 155  ILE A 157 -1  O  ILE A 157   N  ALA A 116
SHEET    3   F 3 PHE A 147  VAL A 149 -1  N  ILE A 148   O  GLN A 156
SHEET    1   G 5 ILE A 201  THR A 205  0
SHEET    2   G 5 GLY A 276  PHE A 287  1  O  PHE A 287   N  ALA A 204
SHEET    3   G 5 ALA A 265  ASN A 273 -1  N  TYR A 267   O  ILE A 282
SHEET    4   G 5 THR A 225  LYS A 230 -1  N  SER A 227   O  ILE A 270
SHEET    5   G 5 GLU A 233  PRO A 234 -1  O  GLU A 233   N  LYS A 230
SSBOND   1 CYS A   22    CYS A   77
SSBOND   2 CYS A  120    CYS A  170
SSBOND   3 CYS A  216    CYS A  269
CISPEP   1 VAL A    6    PRO A    7          0        -0.41
CISPEP   2 THR A  106    PRO A  107          0        -0.64
CISPEP   3 PHE A  221    PRO A  222          0        -0.72
CRYST1   51.440  107.760  149.300  90.00  90.00  90.00 I 21 21 21   8
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
```

Figure 2 (Table 2 (page 8))

```
SCALE1      0.019440  0.000000  0.000000        0.00000
SCALE2      0.000000  0.009280  0.000000        0.00000
SCALE3      0.000000  0.000000  0.006698        0.00000
ATOM      1  N   VAL A  -1      21.197  71.826 -24.060  1.00110.27 N
ATOM      2  CA  VAL A  -1      21.299  70.596 -24.891  1.00112.18 C
ATOM      3  C   VAL A  -1      20.583  69.411 -24.264  1.00111.88 C
ATOM      4  O   VAL A  -1      19.491  69.531 -23.699  1.00113.09 O
ATOM      5  CB  VAL A  -1      22.778  70.161 -25.114  1.00111.00 C
ATOM      6  CG1 VAL A  -1      23.591  71.324 -25.633  1.00109.72 C
ATOM      7  CG2 VAL A  -1      23.374  69.625 -23.817  1.00106.12 C
ATOM      8  N   LEU A   1      21.255  68.270 -24.364  1.00107.51 N
ATOM      9  CA  LEU A   1      20.778  66.981 -23.905  1.00100.28 C
ATOM     10  C   LEU A   1      20.360  66.739 -22.465  1.00 94.24 C
ATOM     11  O   LEU A   1      20.985  67.227 -21.518  1.00 93.77 O
ATOM     12  CB  LEU A   1      21.808  65.936 -24.296  1.00100.43 C
ATOM     13  CG  LEU A   1      21.297  64.909 -25.303  1.00103.11 C
ATOM     14  CD1 LEU A   1      20.253  65.528 -26.233  1.00106.65 C
ATOM     15  CD2 LEU A   1      22.475  64.366 -26.088  1.00101.88 C
ATOM     16  N   GLN A   2      19.299  65.946 -22.328  1.00 87.47 N
ATOM     17  CA  GLN A   2      18.771  65.575 -21.028  1.00 86.76 C
ATOM     18  C   GLN A   2      18.937  64.075 -20.822  1.00 80.18 C
ATOM     19  O   GLN A   2      18.520  63.264 -21.656  1.00 82.58 O
ATOM     20  CB  GLN A   2      17.292  65.950 -20.902  1.00 89.86 C
ATOM     21  CG  GLN A   2      16.819  65.996 -19.458  1.00102.22 C
ATOM     22  CD  GLN A   2      17.932  66.444 -18.500  1.00109.49 C
ATOM     23  OE1 GLN A   2      18.786  67.260 -18.859  1.00112.97 O
ATOM     24  NE2 GLN A   2      17.917  65.917 -17.275  1.00110.51 N
ATOM     25  N   VAL A   3      19.572  63.716 -19.714  1.00 68.44 N
ATOM     26  CA  VAL A   3      19.790  62.317 -19.375  1.00 65.80 C
ATOM     27  C   VAL A   3      19.290  62.058 -17.959  1.00 63.80 C
ATOM     28  O   VAL A   3      19.588  62.816 -17.029  1.00 61.99 O
ATOM     29  CB  VAL A   3      21.291  61.919 -19.495  1.00 70.09 C
ATOM     30  CG1 VAL A   3      22.157  62.831 -18.653  1.00 66.37 C
ATOM     31  CG2 VAL A   3      21.477  60.475 -19.072  1.00 53.43 C
ATOM     32  N   ASP A   4      18.511  60.992 -17.807  1.00 59.47 N
ATOM     33  CA  ASP A   4      17.957  60.635 -16.507  1.00 62.16 C
ATOM     34  C   ASP A   4      18.056  59.137 -16.281  1.00 61.45 C
ATOM     35  O   ASP A   4      17.973  58.337 -17.222  1.00 54.28 O
ATOM     36  CB  ASP A   4      16.490  61.064 -16.410  1.00 57.25 C
ATOM     37  CG  ASP A   4      16.312  62.564 -16.536  1.00 81.12 C
ATOM     38  OD1 ASP A   4      16.784  63.302 -15.644  1.00 87.44 O
ATOM     39  OD2 ASP A   4      15.702  63.010 -17.531  1.00 84.62 O
ATOM     40  N   ILE A   5      18.226  58.760 -15.024  1.00 54.90 N
ATOM     41  CA  ILE A   5      18.324  57.360 -14.692  1.00 47.24 C
ATOM     42  C   ILE A   5      17.134  56.965 -13.832  1.00 49.02 C
ATOM     43  O   ILE A   5      16.846  57.619 -12.826  1.00 47.37 O
ATOM     44  CB  ILE A   5      19.625  57.077 -13.934  1.00 42.30 C
ATOM     45  CG1 ILE A   5      20.823  57.333 -14.849  1.00 48.79 C
ATOM     46  CG2 ILE A   5      19.638  55.615 -13.450  1.00 40.90 C
ATOM     47  CD1 ILE A   5      22.158  57.356 -14.118  1.00 47.66 C
ATOM     48  N   VAL A   6      16.445  55.900 -14.233  1.00 48.39 N
ATOM     49  CA  VAL A   6      15.300  55.401 -13.480  1.00 48.78 C
ATOM     50  C   VAL A   6      15.545  53.939 -13.119  1.00 52.24 C
ATOM     51  O   VAL A   6      15.905  53.130 -13.980  1.00 51.37 O
ATOM     52  CB  VAL A   6      14.008  55.484 -14.299  1.00 55.65 C
ATOM     53  CG1 VAL A   6      12.857  54.882 -13.515  1.00 53.36 C
ATOM     54  CG2 VAL A   6      13.712  56.928 -14.637  1.00 64.21 C
```

Figure 2 (Table 2 (page 9))

ATOM	55	N	PRO	A	7	15.418	53.594	-11.830	1.00	44.55	N
ATOM	56	CA	PRO	A	7	15.074	54.460	-10.692	1.00	44.98	C
ATOM	57	C	PRO	A	7	16.225	55.428	-10.411	1.00	52.07	C
ATOM	58	O	PRO	A	7	17.391	55.112	-10.662	1.00	47.92	O
ATOM	59	CB	PRO	A	7	14.842	53.462	-9.556	1.00	50.48	C
ATOM	60	CG	PRO	A	7	15.718	52.291	-9.944	1.00	45.69	C
ATOM	61	CD	PRO	A	7	15.446	52.181	-11.420	1.00	40.86	C
ATOM	62	N	SER	A	8	15.894	56.604	-9.893	1.00	46.31	N
ATOM	63	CA	SER	A	8	16.889	57.635	-9.634	1.00	49.55	C
ATOM	64	C	SER	A	8	17.921	57.250	-8.592	1.00	53.48	C
ATOM	65	O	SER	A	8	18.995	57.857	-8.515	1.00	54.87	O
ATOM	66	CB	SER	A	8	16.198	58.940	-9.236	1.00	55.09	C
ATOM	67	OG	SER	A	8	15.363	58.753	-8.111	1.00	61.93	O
ATOM	68	N	GLN	A	9	17.597	56.255	-7.776	1.00	46.60	N
ATOM	69	CA	GLN	A	9	18.538	55.781	-6.771	1.00	47.40	C
ATOM	70	C	GLN	A	9	18.204	54.335	-6.448	1.00	44.46	C
ATOM	71	O	GLN	A	9	17.103	53.864	-6.739	1.00	52.34	O
ATOM	72	CB	GLN	A	9	18.494	56.658	-5.515	1.00	58.55	C
ATOM	73	CG	GLN	A	9	17.103	56.860	-4.900	1.00	65.92	C
ATOM	74	CD	GLN	A	9	17.149	57.765	-3.665	1.00	81.94	C
ATOM	75	OE1	GLN	A	9	17.878	57.484	-2.713	1.00	86.13	O
ATOM	76	NE2	GLN	A	9	16.374	58.853	-3.678	1.00	82.96	N
ATOM	77	N	GLY	A	10	19.157	53.606	-5.883	1.00	46.46	N
ATOM	78	CA	GLY	A	10	18.868	52.215	-5.589	1.00	50.99	C
ATOM	79	C	GLY	A	10	19.637	51.600	-4.442	1.00	48.97	C
ATOM	80	O	GLY	A	10	20.719	52.048	-4.070	1.00	46.47	O
ATOM	81	N	GLU	A	11	19.051	50.559	-3.871	1.00	54.04	N
ATOM	82	CA	GLU	A	11	19.684	49.842	-2.778	1.00	54.83	C
ATOM	83	C	GLU	A	11	19.560	48.362	-3.127	1.00	47.65	C
ATOM	84	O	GLU	A	11	18.499	47.918	-3.557	1.00	47.49	O
ATOM	85	CB	GLU	A	11	18.970	50.150	-1.456	1.00	49.30	C
ATOM	86	CG	GLU	A	11	19.627	49.508	-0.255	1.00	67.71	C
ATOM	87	CD	GLU	A	11	19.026	49.974	1.061	1.00	68.83	C
ATOM	88	OE1	GLU	A	11	17.829	49.704	1.305	1.00	70.78	O
ATOM	89	OE2	GLU	A	11	19.758	50.620	1.843	1.00	73.96	O
ATOM	90	N	ILE	A	12	20.636	47.599	-2.965	1.00	44.79	N
ATOM	91	CA	ILE	A	12	20.587	46.178	-3.302	1.00	43.25	C
ATOM	92	C	ILE	A	12	21.164	45.332	-2.185	1.00	49.76	C
ATOM	93	O	ILE	A	12	22.261	45.610	-1.692	1.00	45.49	O
ATOM	94	CB	ILE	A	12	21.402	45.856	-4.562	1.00	46.25	C
ATOM	95	CG1	ILE	A	12	21.182	46.938	-5.621	1.00	48.07	C
ATOM	96	CG2	ILE	A	12	20.984	44.481	-5.114	1.00	40.48	C
ATOM	97	CD1	ILE	A	12	22.125	46.814	-6.795	1.00	44.46	C
ATOM	98	N	SER	A	13	20.421	44.296	-1.796	1.00	50.25	N
ATOM	99	CA	SER	A	13	20.880	43.384	-0.755	1.00	49.85	C
ATOM	100	C	SER	A	13	21.869	42.416	-1.385	1.00	41.84	C
ATOM	101	O	SER	A	13	21.690	41.973	-2.526	1.00	43.99	O
ATOM	102	CB	SER	A	13	19.707	42.608	-0.156	1.00	48.85	C
ATOM	103	OG	SER	A	13	20.157	41.794	0.916	1.00	55.47	O
ATOM	104	N	VAL	A	14	22.926	42.114	-0.644	1.00	50.09	N
ATOM	105	CA	VAL	A	14	23.955	41.214	-1.126	1.00	48.58	C
ATOM	106	C	VAL	A	14	23.358	39.962	-1.742	1.00	53.11	C
ATOM	107	O	VAL	A	14	22.481	39.320	-1.165	1.00	54.25	O
ATOM	108	CB	VAL	A	14	24.924	40.814	0.004	1.00	51.58	C
ATOM	109	CG1	VAL	A	14	25.880	39.739	-0.479	1.00	51.54	C
ATOM	110	CG2	VAL	A	14	25.702	42.027	0.455	1.00	51.93	C
ATOM	111	N	GLY	A	15	23.841	39.636	-2.935	1.00	45.67	N

Figure 2 (Table 2 (page 10))

ATOM	112	CA	GLY	A	15	23.367	38.471	-3.643	1.00	45.80 C
ATOM	113	C	GLY	A	15	22.174	38.738	-4.546	1.00	49.51 C
ATOM	114	O	GLY	A	15	21.845	37.910	-5.395	1.00	44.42 O
ATOM	115	N	GLU	A	16	21.516	39.885	-4.390	1.00	48.69 N
ATOM	116	CA	GLU	A	16	20.360	40.167	-5.239	1.00	44.66 C
ATOM	117	C	GLU	A	16	20.712	41.010	-6.459	1.00	38.83 C
ATOM	118	O	GLU	A	16	21.874	41.355	-6.672	1.00	41.87 O
ATOM	119	CB	GLU	A	16	19.239	40.800	-4.403	1.00	44.40 C
ATOM	120	CG	GLU	A	16	18.799	39.848	-3.289	1.00	57.20 C
ATOM	121	CD	GLU	A	16	17.666	40.373	-2.428	1.00	67.70 C
ATOM	122	OE1	GLU	A	16	17.111	41.448	-2.739	1.00	72.10 O
ATOM	123	OE2	GLU	A	16	17.328	39.695	-1.433	1.00	77.10 O
ATOM	124	N	SER	A	17	19.712	41.319	-7.274	1.00	38.10 N
ATOM	125	CA	SER	A	17	19.950	42.068	-8.496	1.00	39.72 C
ATOM	126	C	SER	A	17	19.039	43.283	-8.655	1.00	43.71 C
ATOM	127	O	SER	A	17	17.960	43.330	-8.074	1.00	48.43 O
ATOM	128	CB	SER	A	17	19.787	41.125	-9.694	1.00	42.04 C
ATOM	129	OG	SER	A	17	20.672	40.016	-9.592	1.00	49.33 O
ATOM	130	N	LYS	A	18	19.491	44.273	-9.427	1.00	39.31 N
ATOM	131	CA	LYS	A	18	18.725	45.495	-9.689	1.00	40.44 C
ATOM	132	C	LYS	A	18	19.194	46.068	-11.004	1.00	36.17 C
ATOM	133	O	LYS	A	18	20.310	45.799	-11.447	1.00	41.18 O
ATOM	134	CB	LYS	A	18	18.944	46.552	-8.603	1.00	45.93 C
ATOM	135	CG	LYS	A	18	17.902	46.558	-7.506	1.00	63.96 C
ATOM	136	CD	LYS	A	18	17.343	47.954	-7.318	1.00	77.99 C
ATOM	137	CE	LYS	A	18	16.408	48.029	-6.120	1.00	91.67 C
ATOM	138	NZ	LYS	A	18	15.285	47.049	-6.198	1.00	104.95 N
ATOM	139	N	PHE	A	19	18.355	46.866	-11.632	1.00	39.73 N
ATOM	140	CA	PHE	A	19	18.758	47.445	-12.889	1.00	42.56 C
ATOM	141	C	PHE	A	19	18.382	48.903	-12.907	1.00	45.52 C
ATOM	142	O	PHE	A	19	17.535	49.352	-12.123	1.00	41.88 O
ATOM	143	CB	PHE	A	19	18.131	46.681	-14.058	1.00	37.12 C
ATOM	144	CG	PHE	A	19	16.658	46.890	-14.220	1.00	41.51 C
ATOM	145	CD1	PHE	A	19	16.175	47.864	-15.090	1.00	45.13 C
ATOM	146	CD2	PHE	A	19	15.742	46.075	-13.547	1.00	42.50 C
ATOM	147	CE1	PHE	A	19	14.794	48.006	-15.310	1.00	44.84 C
ATOM	148	CE2	PHE	A	19	14.377	46.212	-13.759	1.00	43.30 C
ATOM	149	CZ	PHE	A	19	13.899	47.182	-14.639	1.00	41.52 C
ATOM	150	N	PHE	A	20	19.020	49.637	-13.813	1.00	37.54 N
ATOM	151	CA	PHE	A	20	18.816	51.062	-13.938	1.00	38.86 C
ATOM	152	C	PHE	A	20	18.816	51.437	-15.408	1.00	46.44 C
ATOM	153	O	PHE	A	20	19.702	51.035	-16.165	1.00	47.88 O
ATOM	154	CB	PHE	A	20	19.948	51.798	-13.205	1.00	36.96 C
ATOM	155	CG	PHE	A	20	20.112	51.368	-11.784	1.00	46.76 C
ATOM	156	CD1	PHE	A	20	20.904	50.267	-11.460	1.00	48.63 C
ATOM	157	CD2	PHE	A	20	19.427	52.027	-10.765	1.00	42.55 C
ATOM	158	CE1	PHE	A	20	21.008	49.826	-10.138	1.00	46.86 C
ATOM	159	CE2	PHE	A	20	19.525	51.591	-9.436	1.00	40.53 C
ATOM	160	CZ	PHE	A	20	20.317	50.489	-9.126	1.00	44.32 C
ATOM	161	N	LEU	A	21	17.816	52.209	-15.806	1.00	46.01 N
ATOM	162	CA	LEU	A	21	17.680	52.649	-17.189	1.00	49.63 C
ATOM	163	C	LEU	A	21	18.131	54.087	-17.360	1.00	46.97 C
ATOM	164	O	LEU	A	21	17.602	54.990	-16.719	1.00	43.22 O
ATOM	165	CB	LEU	A	21	16.218	52.530	-17.641	1.00	54.55 C
ATOM	166	CG	LEU	A	21	15.857	53.049	-19.040	1.00	57.21 C
ATOM	167	CD1	LEU	A	21	16.625	52.281	-20.096	1.00	58.14 C
ATOM	168	CD2	LEU	A	21	14.365	52.891	-19.274	1.00	55.27 C

Figure 2 (Table 2 (page 11))

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ATOM    169  N   CYS A  22      19.122  54.291 -18.218  1.00 46.45 N
ATOM    170  CA  CYS A  22      19.615  55.628 -18.506  1.00 48.52 C
ATOM    171  C   CYS A  22      18.920  56.056 -19.788  1.00 54.42 C
ATOM    172  O   CYS A  22      19.157  55.478 -20.848  1.00 51.82 O
ATOM    173  CB  CYS A  22      21.115  55.601 -18.730  1.00 49.72 C
ATOM    174  SG  CYS A  22      21.827  57.215 -19.167  1.00 55.16 S
ATOM    175  N   GLN A  23      18.069  57.071 -19.689  1.00 59.11 N
ATOM    176  CA  GLN A  23      17.312  57.546 -20.837  1.00 66.68 C
ATOM    177  C   GLN A  23      17.718  58.941 -21.314  1.00 63.21 C
ATOM    178  O   GLN A  23      17.951  59.839 -20.509  1.00 57.50 O
ATOM    179  CB  GLN A  23      15.825  57.547 -20.482  1.00 69.27 C
ATOM    180  CG  GLN A  23      14.900  57.940 -21.618  1.00 83.38 C
ATOM    181  CD  GLN A  23      14.575  56.779 -22.549  1.00 90.68 C
ATOM    182  OE1 GLN A  23      14.251  55.685 -22.089  1.00 97.59 O
ATOM    183  NE2 GLN A  23      14.642  57.016 -23.861  1.00 95.34 N
ATOM    184  N   VAL A  24      17.799  59.118 -22.629  1.00 67.26 N
ATOM    185  CA  VAL A  24      18.145  60.415 -23.197  1.00 74.82 C
ATOM    186  C   VAL A  24      16.857  61.028 -23.739  1.00 75.90 C
ATOM    187  O   VAL A  24      16.039  60.338 -24.356  1.00 76.41 O
ATOM    188  CB  VAL A  24      19.178  60.285 -24.343  1.00 77.43 C
ATOM    189  CG1 VAL A  24      19.560  61.657 -24.852  1.00 77.38 C
ATOM    190  CG2 VAL A  24      20.418  59.547 -23.856  1.00 81.07 C
ATOM    191  N   ALA A  25      16.685  62.324 -23.500  1.00 82.73 N
ATOM    192  CA  ALA A  25      15.490  63.053 -23.933  1.00 92.22 C
ATOM    193  C   ALA A  25      15.455  63.428 -25.424  1.00 99.21 C
ATOM    194  O   ALA A  25      16.491  63.734 -26.019  1.00 99.63 O
ATOM    195  CB  ALA A  25      15.326  64.307 -23.078  1.00 89.44 C
ATOM    196  N   GLY A  26      14.249  63.405 -26.002  1.00107.66 N
ATOM    197  CA  GLY A  26      14.040  63.735 -27.410  1.00117.13 C
ATOM    198  C   GLY A  26      14.697  62.739 -28.348  1.00123.74 C
ATOM    199  O   GLY A  26      14.060  62.088 -29.188  1.00126.85 O
ATOM    200  N   ASP A  27      16.010  62.671 -28.187  1.00127.93 N
ATOM    201  CA  ASP A  27      16.915  61.795 -28.897  1.00131.73 C
ATOM    202  C   ASP A  27      17.049  61.809 -30.410  1.00132.38 C
ATOM    203  O   ASP A  27      16.518  60.944 -31.112  1.00134.43 O
ATOM    204  CB  ASP A  27      16.721  60.353 -28.433  1.00133.67 C
ATOM    205  CG  ASP A  27      17.976  59.540 -28.620  1.00136.05 C
ATOM    206  OD1 ASP A  27      19.011  60.177 -28.888  1.00137.46 O
ATOM    207  OD2 ASP A  27      17.940  58.305 -28.501  1.00138.22 O
ATOM    208  N   ALA A  28      17.776  62.812 -30.894  1.00130.01 N
ATOM    209  CA  ALA A  28      18.098  62.888 -32.301  1.00127.19 C
ATOM    210  C   ALA A  28      19.203  61.826 -32.208  1.00125.97 C
ATOM    211  O   ALA A  28      19.562  61.453 -31.091  1.00125.76 O
ATOM    212  CB  ALA A  28      18.672  64.248 -32.657  1.00123.21 C
ATOM    213  N   LYS A  29      19.777  61.332 -33.300  1.00124.23 N
ATOM    214  CA  LYS A  29      20.754  60.267 -33.095  1.00120.04 C
ATOM    215  C   LYS A  29      22.237  60.419 -33.356  1.00114.93 C
ATOM    216  O   LYS A  29      22.773  61.503 -33.593  1.00109.02 O
ATOM    217  CB  LYS A  29      20.254  58.988 -33.777  1.00124.97 C
ATOM    218  CG  LYS A  29      19.095  58.340 -33.030  1.00125.66 C
ATOM    219  CD  LYS A  29      18.639  57.047 -33.674  1.00125.32 C
ATOM    220  CE  LYS A  29      17.462  56.460 -32.915  1.00120.15 C
ATOM    221  NZ  LYS A  29      16.388  57.477 -32.740  1.00120.03 N
ATOM    222  N   ASP A  30      22.875  59.260 -33.286  1.00110.94 N
ATOM    223  CA  ASP A  30      24.297  59.108 -33.440  1.00108.72 C
ATOM    224  C   ASP A  30      25.004  59.738 -32.257  1.00102.56 C
ATOM    225  O   ASP A  30      25.869  60.592 -32.425  1.00101.55 O
```

Figure 2 (Table 2 (page 12))

```
ATOM    226  CB  ASP A  30      24.800  59.729 -34.740  1.00114.65 C
ATOM    227  CG  ASP A  30      25.573  58.735 -35.584  1.00121.84 C
ATOM    228  OD1 ASP A  30      26.219  57.833 -35.001  1.00126.50 O
ATOM    229  OD2 ASP A  30      25.543  58.853 -36.824  1.00125.16 O
ATOM    230  N   LYS A  31      24.602  59.339 -31.055  1.00 90.62 N
ATOM    231  CA  LYS A  31      25.252  59.820 -29.845  1.00 86.82 C
ATOM    232  C   LYS A  31      25.645  58.547 -29.120  1.00 76.37 C
ATOM    233  O   LYS A  31      25.000  57.512 -29.280  1.00 76.59 O
ATOM    234  CB  LYS A  31      24.315  60.658 -28.965  1.00 87.55 C
ATOM    235  CG  LYS A  31      23.238  59.873 -28.261  1.00 90.62 C
ATOM    236  CD  LYS A  31      21.906  60.210 -28.856  1.00 90.82 C
ATOM    237  CE  LYS A  31      21.081  58.968 -28.999  1.00 94.15 C
ATOM    238  NZ  LYS A  31      20.424  58.901 -30.339  1.00 96.17 N
ATOM    239  N   ASP A  32      26.711  58.620 -28.341  1.00 66.33 N
ATOM    240  CA  ASP A  32      27.202  57.467 -27.607  1.00 64.69 C
ATOM    241  C   ASP A  32      26.732  57.503 -26.163  1.00 57.45 C
ATOM    242  O   ASP A  32      26.707  58.563 -25.532  1.00 61.27 O
ATOM    243  CB  ASP A  32      28.740  57.448 -27.669  1.00 59.49 C
ATOM    244  CG  ASP A  32      29.372  56.362 -26.791  1.00 67.93 C
ATOM    245  OD1 ASP A  32      29.627  56.626 -25.589  1.00 51.53 O
ATOM    246  OD2 ASP A  32      29.626  55.248 -27.308  1.00 61.79 O
ATOM    247  N   ILE A  33      26.336  56.342 -25.657  1.00 54.91 N
ATOM    248  CA  ILE A  33      25.911  56.210 -24.271  1.00 52.46 C
ATOM    249  C   ILE A  33      26.823  55.173 -23.640  1.00 53.58 C
ATOM    250  O   ILE A  33      26.875  54.022 -24.083  1.00 50.96 O
ATOM    251  CB  ILE A  33      24.470  55.712 -24.139  1.00 51.31 C
ATOM    252  CG1 ILE A  33      23.518  56.700 -24.800  1.00 52.96 C
ATOM    253  CG2 ILE A  33      24.116  55.563 -22.654  1.00 50.09 C
ATOM    254  CD1 ILE A  33      22.087  56.233 -24.828  1.00 54.31 C
ATOM    255  N   SER A  34      27.535  55.588 -22.603  1.00 43.80 N
ATOM    256  CA  SER A  34      28.463  54.716 -21.910  1.00 47.69 C
ATOM    257  C   SER A  34      28.262  54.831 -20.410  1.00 51.46 C
ATOM    258  O   SER A  34      27.899  55.892 -19.897  1.00 50.26 O
ATOM    259  CB  SER A  34      29.898  55.105 -22.255  1.00 44.86 C
ATOM    260  OG  SER A  34      30.197  54.768 -23.592  1.00 56.99 O
ATOM    261  N   TRP A  35      28.488  53.726 -19.714  1.00 47.72 N
ATOM    262  CA  TRP A  35      28.359  53.713 -18.270  1.00 42.75 C
ATOM    263  C   TRP A  35      29.741  53.598 -17.652  1.00 45.12 C
ATOM    264  O   TRP A  35      30.640  52.967 -18.223  1.00 44.07 O
ATOM    265  CB  TRP A  35      27.511  52.531 -17.800  1.00 39.02 C
ATOM    266  CG  TRP A  35      26.028  52.667 -18.015  1.00 43.96 C
ATOM    267  CD1 TRP A  35      25.323  52.308 -19.126  1.00 38.82 C
ATOM    268  CD2 TRP A  35      25.062  53.080 -17.041  1.00 36.18 C
ATOM    269  NE1 TRP A  35      23.974  52.454 -18.901  1.00 45.99 N
ATOM    270  CE2 TRP A  35      23.786  52.925 -17.632  1.00 47.03 C
ATOM    271  CE3 TRP A  35      25.150  53.556 -15.735  1.00 39.81 C
ATOM    272  CZ2 TRP A  35      22.605  53.232 -16.948  1.00 43.25 C
ATOM    273  CZ3 TRP A  35      23.962  53.865 -15.054  1.00 41.38 C
ATOM    274  CH2 TRP A  35      22.713  53.699 -15.668  1.00 42.80 C
ATOM    275  N   PHE A  36      29.907  54.225 -16.491  1.00 45.19 N
ATOM    276  CA  PHE A  36      31.160  54.178 -15.748  1.00 44.89 C
ATOM    277  C   PHE A  36      30.834  53.716 -14.345  1.00 44.82 C
ATOM    278  O   PHE A  36      29.858  54.166 -13.755  1.00 41.52 O
ATOM    279  CB  PHE A  36      31.819  55.556 -15.675  1.00 43.10 C
ATOM    280  CG  PHE A  36      32.286  56.062 -17.006  1.00 55.53 C
ATOM    281  CD1 PHE A  36      31.385  56.639 -17.893  1.00 51.14 C
ATOM    282  CD2 PHE A  36      33.610  55.883 -17.407  1.00 46.89 C
```

Figure 2 (Table 2 (page 13))

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ATOM    283  CE1 PHE A  36      31.789  57.030 -19.173  1.00 54.91 C
ATOM    284  CE2 PHE A  36      34.030  56.269 -18.684  1.00 55.64 C
ATOM    285  CZ  PHE A  36      33.110  56.846 -19.573  1.00 50.29 C
ATOM    286  N   SER A  37      31.641  52.795 -13.832  1.00 42.90 N
ATOM    287  CA  SER A  37      31.447  52.289 -12.488  1.00 52.59 C
ATOM    288  C   SER A  37      31.973  53.321 -11.490  1.00 53.66 C
ATOM    289  O   SER A  37      32.581  54.325 -11.878  1.00 46.56 O
ATOM    290  CB  SER A  37      32.176  50.950 -12.322  1.00 56.49 C
ATOM    291  OG  SER A  37      33.540  51.055 -12.675  1.00 54.60 O
ATOM    292  N   PRO A  38      31.729  53.096 -10.192  1.00 55.82 N
ATOM    293  CA  PRO A  38      32.169  54.004  -9.124  1.00 58.18 C
ATOM    294  C   PRO A  38      33.682  54.241  -9.057  1.00 56.07 C
ATOM    295  O   PRO A  38      34.135  55.248  -8.519  1.00 57.12 O
ATOM    296  CB  PRO A  38      31.619  53.338  -7.864  1.00 55.81 C
ATOM    297  CG  PRO A  38      30.327  52.731  -8.377  1.00 51.53 C
ATOM    298  CD  PRO A  38      30.764  52.107  -9.677  1.00 50.32 C
ATOM    299  N   ASN A  39      34.456  53.317  -9.609  1.00 52.69 N
ATOM    300  CA  ASN A  39      35.905  53.452  -9.613  1.00 59.02 C
ATOM    301  C   ASN A  39      36.396  54.175 -10.881  1.00 61.73 C
ATOM    302  O   ASN A  39      37.585  54.160 -11.188  1.00 57.13 O
ATOM    303  CB  ASN A  39      36.551  52.077  -9.523  1.00 56.75 C
ATOM    304  CG  ASN A  39      36.432  51.310 -10.810  1.00 71.38 C
ATOM    305  OD1 ASN A  39      35.531  51.565 -11.603  1.00 73.88 O
ATOM    306  ND2 ASN A  39      37.332  50.361 -11.027  1.00 79.44 N
ATOM    307  N   GLY A  40      35.471  54.777 -11.626  1.00 54.18 N
ATOM    308  CA  GLY A  40      35.839  55.523 -12.825  1.00 58.26 C
ATOM    309  C   GLY A  40      36.049  54.777 -14.126  1.00 56.72 C
ATOM    310  O   GLY A  40      36.311  55.385 -15.161  1.00 59.14 O
ATOM    311  N   GLU A  41      35.940  53.462 -14.098  1.00 53.24 N
ATOM    312  CA  GLU A  41      36.137  52.712 -15.312  1.00 54.15 C
ATOM    313  C   GLU A  41      34.887  52.572 -16.152  1.00 52.64 C
ATOM    314  O   GLU A  41      33.772  52.444 -15.645  1.00 51.92 O
ATOM    315  CB  GLU A  41      36.695  51.341 -14.988  1.00 62.00 C
ATOM    316  CG  GLU A  41      38.100  51.410 -14.451  1.00 86.56 C
ATOM    317  CD  GLU A  41      38.565  50.074 -13.931  1.00 94.84 C
ATOM    318  OE1 GLU A  41      37.901  49.059 -14.243  1.00 99.92 O
ATOM    319  OE2 GLU A  41      39.591  50.041 -13.220  1.00 98.17 O
ATOM    320  N   LYS A  42      35.104  52.625 -17.457  1.00 48.52 N
ATOM    321  CA  LYS A  42      34.050  52.475 -18.430  1.00 45.24 C
ATOM    322  C   LYS A  42      33.714  50.979 -18.477  1.00 52.84 C
ATOM    323  O   LYS A  42      34.607  50.126 -18.534  1.00 47.42 O
ATOM    324  CB  LYS A  42      34.536  52.971 -19.796  1.00 46.19 C
ATOM    325  CG  LYS A  42      33.502  52.863 -20.930  1.00 58.73 C
ATOM    326  CD  LYS A  42      34.006  53.553 -22.205  1.00 60.30 C
ATOM    327  CE  LYS A  42      33.004  53.446 -23.353  1.00 69.24 C
ATOM    328  NZ  LYS A  42      33.486  54.104 -24.606  1.00 73.95 N
ATOM    329  N   LEU A  43      32.425  50.659 -18.441  1.00 42.58 N
ATOM    330  CA  LEU A  43      31.986  49.270 -18.453  1.00 44.33 C
ATOM    331  C   LEU A  43      31.907  48.724 -19.863  1.00 45.36 C
ATOM    332  O   LEU A  43      31.315  49.351 -20.734  1.00 49.42 O
ATOM    333  CB  LEU A  43      30.613  49.177 -17.778  1.00 37.59 C
ATOM    334  CG  LEU A  43      30.672  49.579 -16.302  1.00 45.02 C
ATOM    335  CD1 LEU A  43      29.276  49.708 -15.713  1.00 48.59 C
ATOM    336  CD2 LEU A  43      31.489  48.538 -15.550  1.00 45.09 C
ATOM    337  N   SER A  44      32.507  47.566 -20.100  0.50 34.43 N
ATOM    338  CA  SER A  44      32.436  46.990 -21.429  0.50 37.54 C
ATOM    339  C   SER A  44      31.017  46.509 -21.595  0.50 40.70 C
```

Figure 2 (Table 2 (page 14))

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ATOM    340  O   SER A  44      30.404  45.984 -20.672  0.50 31.07 O
ATOM    341  CB  SER A  44      33.394  45.813 -21.590  0.50 34.76 C
ATOM    342  OG  SER A  44      34.730  46.238 -21.418  0.50 37.63 O
ATOM    343  N   PRO A  45      30.475  46.684 -22.787  1.00 55.79 N
ATOM    344  CA  PRO A  45      29.104  46.261 -23.062  1.00 56.53 C
ATOM    345  C   PRO A  45      28.910  44.761 -23.041  1.00 53.37 C
ATOM    346  O   PRO A  45      29.849  43.986 -23.229  1.00 56.21 O
ATOM    347  CB  PRO A  45      28.836  46.833 -24.458  1.00 60.37 C
ATOM    348  CG  PRO A  45      29.823  47.960 -24.586  1.00 60.02 C
ATOM    349  CD  PRO A  45      31.056  47.392 -23.941  1.00 63.21 C
ATOM    350  N   ASN A  46      27.667  44.370 -22.800  1.00 57.48 N
ATOM    351  CA  ASN A  46      27.279  42.973 -22.812  1.00 57.72 C
ATOM    352  C   ASN A  46      28.150  41.993 -22.017  1.00 57.75 C
ATOM    353  O   ASN A  46      28.534  40.950 -22.541  1.00 60.65 O
ATOM    354  CB  ASN A  46      27.179  42.508 -24.272  1.00 67.80 C
ATOM    355  CG  ASN A  46      26.285  43.417 -25.119  1.00 71.96 C
ATOM    356  OD1 ASN A  46      25.090  43.557 -24.850  1.00 81.33 O
ATOM    357  ND2 ASN A  46      26.862  44.033 -26.146  1.00 70.84 N
ATOM    358  N   GLN A  47      28.478  42.325 -20.771  1.00 53.34 N
ATOM    359  CA  GLN A  47      29.250  41.408 -19.925  1.00 49.41 C
ATOM    360  C   GLN A  47      28.202  40.672 -19.091  1.00 50.32 C
ATOM    361  O   GLN A  47      27.029  41.040 -19.111  1.00 47.47 O
ATOM    362  CB  GLN A  47      30.232  42.156 -19.022  1.00 51.46 C
ATOM    363  CG  GLN A  47      31.291  42.936 -19.798  1.00 49.02 C
ATOM    364  CD  GLN A  47      32.023  42.055 -20.812  1.00 60.54 C
ATOM    365  OE1 GLN A  47      32.910  41.286 -20.448  1.00 52.30 O
ATOM    366  NE2 GLN A  47      31.634  42.149 -22.082  1.00 51.19 N
ATOM    367  N   GLN A  48      28.630  39.669 -18.336  1.00 52.29 N
ATOM    368  CA  GLN A  48      27.728  38.807 -17.566  1.00 56.49 C
ATOM    369  C   GLN A  48      27.049  39.337 -16.305  1.00 58.23 C
ATOM    370  O   GLN A  48      25.818  39.453 -16.238  1.00 50.89 O
ATOM    371  CB  GLN A  48      28.486  37.524 -17.199  1.00 69.79 C
ATOM    372  CG  GLN A  48      27.606  36.324 -16.903  1.00 85.42 C
ATOM    373  CD  GLN A  48      27.071  35.675 -18.172  1.00 96.52 C
ATOM    374  OE1 GLN A  48      27.848  35.302 -19.052  1.00103.65 O
ATOM    375  NE2 GLN A  48      25.745  35.530 -18.272  1.00 97.26 N
ATOM    376  N   ARG A  49      27.866  39.613 -15.297  1.00 46.27 N
ATOM    377  CA  ARG A  49      27.376  40.069 -14.009  1.00 49.02 C
ATOM    378  C   ARG A  49      27.031  41.558 -13.965  1.00 50.34 C
ATOM    379  O   ARG A  49      25.951  41.929 -13.518  1.00 44.46 O
ATOM    380  CB  ARG A  49      28.404  39.724 -12.937  1.00 43.05 C
ATOM    381  CG  ARG A  49      27.841  39.691 -11.541  1.00 50.00 C
ATOM    382  CD  ARG A  49      28.920  39.301 -10.560  1.00 46.14 C
ATOM    383  NE  ARG A  49      29.847  40.402 -10.332  1.00 50.29 N
ATOM    384  CZ  ARG A  49      29.552  41.479  -9.614  1.00 49.75 C
ATOM    385  NH1 ARG A  49      28.355  41.602  -9.054  1.00 46.61 N
ATOM    386  NH2 ARG A  49      30.456  42.434  -9.450  1.00 54.16 N
ATOM    387  N   ILE A  50      27.950  42.413 -14.404  1.00 45.13 N
ATOM    388  CA  ILE A  50      27.693  43.846 -14.431  1.00 47.45 C
ATOM    389  C   ILE A  50      27.362  44.081 -15.886  1.00 49.10 C
ATOM    390  O   ILE A  50      28.236  44.288 -16.718  1.00 46.05 O
ATOM    391  CB  ILE A  50      28.927  44.633 -13.989  1.00 46.67 C
ATOM    392  CG1 ILE A  50      29.309  44.197 -12.569  1.00 49.39 C
ATOM    393  CG2 ILE A  50      28.645  46.122 -14.047  1.00 45.96 C
ATOM    394  CD1 ILE A  50      28.175  44.305 -11.547  1.00 38.44 C
ATOM    395  N   SER A  51      26.069  44.019 -16.172  1.00 45.97 N
ATOM    396  CA  SER A  51      25.572  44.111 -17.523  1.00 42.85 C
```

Figure 2 (Table 2 (page 15))

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ATOM    397  C   SER A  51      25.123  45.464 -18.027  1.00 47.59 C
ATOM    398  O   SER A  51      24.300  46.145 -17.408  1.00 47.20 O
ATOM    399  CB  SER A  51      24.430  43.096 -17.676  1.00 42.67 C
ATOM    400  OG  SER A  51      23.643  43.375 -18.811  1.00 55.89 O
ATOM    401  N   VAL A  52      25.689  45.856 -19.159  1.00 45.49 N
ATOM    402  CA  VAL A  52      25.317  47.100 -19.802  1.00 46.68 C
ATOM    403  C   VAL A  52      24.768  46.706 -21.155  1.00 52.16 C
ATOM    404  O   VAL A  52      25.483  46.140 -21.991  1.00 52.43 O
ATOM    405  CB  VAL A  52      26.504  48.038 -20.028  1.00 51.87 C
ATOM    406  CG1 VAL A  52      26.064  49.202 -20.901  1.00 49.68 C
ATOM    407  CG2 VAL A  52      27.029  48.555 -18.694  1.00 46.22 C
ATOM    408  N   VAL A  53      23.491  46.999 -21.353  1.00 43.80 N
ATOM    409  CA  VAL A  53      22.813  46.679 -22.584  1.00 51.71 C
ATOM    410  C   VAL A  53      22.126  47.901 -23.192  1.00 60.49 C
ATOM    411  O   VAL A  53      21.288  48.550 -22.564  1.00 55.82 O
ATOM    412  CB  VAL A  53      21.770  45.573 -22.343  1.00 57.05 C
ATOM    413  CG1 VAL A  53      20.897  45.392 -23.569  1.00 61.58 C
ATOM    414  CG2 VAL A  53      22.478  44.269 -22.008  1.00 51.45 C
ATOM    415  N   TRP A  54      22.511  48.205 -24.422  1.00 65.48 N
ATOM    416  CA  TRP A  54      21.948  49.309 -25.178  1.00 74.11 C
ATOM    417  C   TRP A  54      20.581  48.813 -25.650  1.00 74.48 C
ATOM    418  O   TRP A  54      20.475  47.706 -26.167  1.00 72.95 O
ATOM    419  CB  TRP A  54      22.851  49.571 -26.365  1.00 82.17 C
ATOM    420  CG  TRP A  54      22.565  50.791 -27.135  1.00 99.79 C
ATOM    421  CD1 TRP A  54      22.877  52.073 -26.787  1.00102.50 C
ATOM    422  CD2 TRP A  54      22.021  50.849 -28.456  1.00107.53 C
ATOM    423  NE1 TRP A  54      22.573  52.929 -27.817  1.00109.34 N
ATOM    424  CE2 TRP A  54      22.045  52.205 -28.852  1.00111.35 C
ATOM    425  CE3 TRP A  54      21.515  49.889 -29.343  1.00108.73 C
ATOM    426  CZ2 TRP A  54      21.590  52.619 -30.108  1.00112.86 C
ATOM    427  CZ3 TRP A  54      21.061  50.305 -30.591  1.00109.55 C
ATOM    428  CH2 TRP A  54      21.100  51.662 -30.959  1.00110.38 C
ATOM    429  N   ASN A  55      19.537  49.612 -25.471  1.00 71.63 N
ATOM    430  CA  ASN A  55      18.205  49.185 -25.878  1.00 76.76 C
ATOM    431  C   ASN A  55      17.845  49.651 -27.281  1.00 81.91 C
ATOM    432  O   ASN A  55      17.573  48.846 -28.168  1.00 88.33 O
ATOM    433  CB  ASN A  55      17.197  49.689 -24.858  1.00 71.55 C
ATOM    434  CG  ASN A  55      17.474  49.141 -23.476  1.00 75.04 C
ATOM    435  OD1 ASN A  55      17.374  47.932 -23.246  1.00 72.25 O
ATOM    436  ND2 ASN A  55      17.841  50.021 -22.550  1.00 50.95 N
ATOM    437  N   ASP A  56      17.833  50.962 -27.455  1.00 88.42 N
ATOM    438  CA  ASP A  56      17.548  51.607 -28.722  1.00 96.25 C
ATOM    439  C   ASP A  56      18.566  52.727 -28.677  1.00101.81 C
ATOM    440  O   ASP A  56      19.369  52.797 -27.736  1.00102.77 O
ATOM    441  CB  ASP A  56      16.107  52.147 -28.744  1.00 95.48 C
ATOM    442  CG  ASP A  56      15.707  52.811 -27.433  1.00 93.76 C
ATOM    443  OD1 ASP A  56      16.451  53.704 -26.985  1.00 85.05 O
ATOM    444  OD2 ASP A  56      14.658  52.452 -26.849  1.00 93.98 O
ATOM    445  N   ASP A  57      18.599  53.607 -29.663  1.00102.50 N
ATOM    446  CA  ASP A  57      19.610  54.674 -29.562  1.00102.11 C
ATOM    447  C   ASP A  57      19.218  55.678 -28.491  1.00 97.41 C
ATOM    448  O   ASP A  57      19.933  56.652 -28.258  1.00 97.40 O
ATOM    449  CB  ASP A  57      19.781  55.395 -30.900  1.00112.19 C
ATOM    450  CG  ASP A  57      21.068  56.116 -30.995  1.00121.70 C
ATOM    451  OD1 ASP A  57      21.660  56.543 -29.959  1.00128.34 O
ATOM    452  OD2 ASP A  57      21.589  56.364 -32.125  1.00123.94 O
ATOM    453  N   ASP A  58      18.084  55.433 -27.843  1.00 90.49 N
```

Figure 2 (Table 2 (page 16))

```
ATOM    454  CA  ASP A  58      17.622  56.352 -26.826  1.00 87.06 C
ATOM    455  C   ASP A  58      18.071  55.997 -25.427  1.00 73.82 C
ATOM    456  O   ASP A  58      18.180  56.880 -24.577  1.00 62.84 O
ATOM    457  CB  ASP A  58      16.093  56.433 -26.809  1.00103.58 C
ATOM    458  CG  ASP A  58      15.487  56.564 -28.191  1.00113.84 C
ATOM    459  OD1 ASP A  58      15.498  57.677 -28.763  1.00117.69 O
ATOM    460  OD2 ASP A  58      14.997  55.534 -28.700  1.00121.72 O
ATOM    461  N   SER A  59      18.320  54.717 -25.174  1.00 64.75 N
ATOM    462  CA  SER A  59      18.681  54.313 -23.828  1.00 61.90 C
ATOM    463  C   SER A  59      19.628  53.131 -23.689  1.00 64.15 C
ATOM    464  O   SER A  59      19.869  52.359 -24.627  1.00 60.43 O
ATOM    465  CB  SER A  59      17.408  54.000 -23.052  1.00 55.02 C
ATOM    466  OG  SER A  59      16.760  52.881 -23.625  1.00 62.54 O
ATOM    467  N   SER A  60      20.145  53.005 -22.473  1.00 58.32 N
ATOM    468  CA  SER A  60      21.062  51.941 -22.111  1.00 53.12 C
ATOM    469  C   SER A  60      20.694  51.465 -20.708  1.00 51.38 C
ATOM    470  O   SER A  60      20.439  52.271 -19.815  1.00 50.11 O
ATOM    471  CB  SER A  60      22.502  52.451 -22.127  1.00 48.06 C
ATOM    472  OG  SER A  60      23.407  51.420 -21.751  1.00 54.93 O
ATOM    473  N   THR A  61      20.667  50.157 -20.509  1.00 41.41 N
ATOM    474  CA  THR A  61      20.308  49.618 -19.206  1.00 44.19 C
ATOM    475  C   THR A  61      21.489  48.979 -18.501  1.00 42.41 C
ATOM    476  O   THR A  61      22.227  48.188 -19.081  1.00 46.93 O
ATOM    477  CB  THR A  61      19.183  48.583 -19.353  1.00 47.49 C
ATOM    478  OG1 THR A  61      18.023  49.233 -19.880  1.00 56.06 O
ATOM    479  CG2 THR A  61      18.837  47.945 -18.004  1.00 45.18 C
ATOM    480  N   LEU A  62      21.674  49.359 -17.247  1.00 37.61 N
ATOM    481  CA  LEU A  62      22.731  48.797 -16.432  1.00 39.04 C
ATOM    482  C   LEU A  62      22.076  47.810 -15.475  1.00 38.19 C
ATOM    483  O   LEU A  62      21.171  48.185 -14.722  1.00 38.43 O
ATOM    484  CB  LEU A  62      23.431  49.896 -15.628  1.00 34.82 C
ATOM    485  CG  LEU A  62      24.273  49.373 -14.461  1.00 46.86 C
ATOM    486  CD1 LEU A  62      25.418  48.550 -14.996  1.00 41.11 C
ATOM    487  CD2 LEU A  62      24.797  50.517 -13.617  1.00 40.98 C
ATOM    488  N   THR A  63      22.488  46.548 -15.514  1.00 34.32 N
ATOM    489  CA  THR A  63      21.930  45.570 -14.583  1.00 42.11 C
ATOM    490  C   THR A  63      23.043  45.058 -13.694  1.00 38.02 C
ATOM    491  O   THR A  63      24.086  44.634 -14.181  1.00 39.91 O
ATOM    492  CB  THR A  63      21.312  44.333 -15.284  1.00 44.60 C
ATOM    493  OG1 THR A  63      20.291  44.746 -16.193  1.00 38.13 O
ATOM    494  CG2 THR A  63      20.709  43.388 -14.247  1.00 41.53 C
ATOM    495  N   ILE A  64      22.831  45.096 -12.390  1.00 32.30 N
ATOM    496  CA  ILE A  64      23.835  44.596 -11.464  1.00 40.27 C
ATOM    497  C   ILE A  64      23.288  43.299 -10.884  1.00 44.61 C
ATOM    498  O   ILE A  64      22.400  43.324 -10.032  1.00 43.38 O
ATOM    499  CB  ILE A  64      24.116  45.600 -10.319  1.00 43.07 C
ATOM    500  CG1 ILE A  64      24.757  46.868 -10.894  1.00 50.00 C
ATOM    501  CG2 ILE A  64      25.032  44.962  -9.265  1.00 36.35 C
ATOM    502  CD1 ILE A  64      25.080  47.930  -9.867  1.00 45.66 C
ATOM    503  N   TYR A  65      23.811  42.175 -11.373  1.00 41.50 N
ATOM    504  CA  TYR A  65      23.398  40.851 -10.917  1.00 41.75 C
ATOM    505  C   TYR A  65      24.239  40.399  -9.746  1.00 46.17 C
ATOM    506  O   TYR A  65      25.400  40.796  -9.628  1.00 46.44 O
ATOM    507  CB  TYR A  65      23.591  39.814 -12.023  1.00 39.24 C
ATOM    508  CG  TYR A  65      22.643  39.936 -13.177  1.00 46.02 C
ATOM    509  CD1 TYR A  65      23.074  40.408 -14.415  1.00 43.20 C
ATOM    510  CD2 TYR A  65      21.304  39.560 -13.035  1.00 40.19 C
```

Figure 2 (Table 2 (page 17))

```
ATOM    511  CE1 TYR A  65      22.198  40.503 -15.492  1.00 46.92 C
ATOM    512  CE2 TYR A  65      20.406  39.644 -14.117  1.00 42.02 C
ATOM    513  CZ  TYR A  65      20.868  40.117 -15.337  1.00 47.29 C
ATOM    514  OH  TYR A  65      20.008  40.185 -16.399  1.00 46.88 O
ATOM    515  N   ASN A  66      23.660  39.556  -8.897  1.00 43.81 N
ATOM    516  CA  ASN A  66      24.368  38.990  -7.756  1.00 48.17 C
ATOM    517  C   ASN A  66      25.277  40.002  -7.062  1.00 48.24 C
ATOM    518  O   ASN A  66      26.489  39.792  -6.955  1.00 48.04 O
ATOM    519  CB  ASN A  66      25.206  37.817  -8.241  1.00 44.79 C
ATOM    520  CG  ASN A  66      25.844  37.052  -7.100  1.00 58.80 C
ATOM    521  OD1 ASN A  66      26.868  36.393  -7.279  1.00 62.64 O
ATOM    522  ND2 ASN A  66      25.237  37.127  -5.919  1.00 60.17 N
ATOM    523  N   ALA A  67      24.684  41.080  -6.566  1.00 47.68 N
ATOM    524  CA  ALA A  67      25.448  42.151  -5.935  1.00 40.81 C
ATOM    525  C   ALA A  67      26.301  41.798  -4.739  1.00 49.08 C
ATOM    526  O   ALA A  67      25.937  40.963  -3.910  1.00 47.57 O
ATOM    527  CB  ALA A  67      24.523  43.290  -5.553  1.00 44.48 C
ATOM    528  N   ASN A  68      27.435  42.482  -4.649  1.00 50.95 N
ATOM    529  CA  ASN A  68      28.344  42.315  -3.529  1.00 54.43 C
ATOM    530  C   ASN A  68      28.763  43.719  -3.093  1.00 55.80 C
ATOM    531  O   ASN A  68      28.665  44.678  -3.872  1.00 45.45 O
ATOM    532  CB  ASN A  68      29.557  41.476  -3.922  1.00 51.73 C
ATOM    533  CG  ASN A  68      30.494  42.201  -4.854  1.00 61.49 C
ATOM    534  OD1 ASN A  68      30.920  43.322  -4.579  1.00 60.88 O
ATOM    535  ND2 ASN A  68      30.835  41.554  -5.963  1.00 52.62 N
ATOM    536  N   ILE A  69      29.235  43.835  -1.856  1.00 52.73 N
ATOM    537  CA  ILE A  69      29.630  45.118  -1.285  1.00 58.71 C
ATOM    538  C   ILE A  69      30.545  45.990  -2.137  1.00 51.79 C
ATOM    539  O   ILE A  69      30.483  47.208  -2.043  1.00 52.79 O
ATOM    540  CB  ILE A  69      30.299  44.937   0.095  1.00 60.50 C
ATOM    541  CG1 ILE A  69      31.681  44.301  -0.063  1.00 67.17 C
ATOM    542  CG2 ILE A  69      29.410  44.091   0.987  1.00 59.59 C
ATOM    543  CD1 ILE A  69      32.506  44.314   1.211  1.00 80.29 C
ATOM    544  N   ASP A  70      31.396  45.384  -2.956  1.00 46.36 N
ATOM    545  CA  ASP A  70      32.277  46.184  -3.781  1.00 50.45 C
ATOM    546  C   ASP A  70      31.587  46.792  -4.991  1.00 58.77 C
ATOM    547  O   ASP A  70      32.227  47.477  -5.784  1.00 53.61 O
ATOM    548  CB  ASP A  70      33.473  45.369  -4.241  1.00 50.41 C
ATOM    549  CG  ASP A  70      34.388  44.991  -3.088  1.00 69.82 C
ATOM    550  OD1 ASP A  70      34.622  45.851  -2.208  1.00 68.65 O
ATOM    551  OD2 ASP A  70      34.878  43.842  -3.064  1.00 67.67 O
ATOM    552  N   ASP A  71      30.290  46.540  -5.144  1.00 54.09 N
ATOM    553  CA  ASP A  71      29.554  47.102  -6.269  1.00 50.10 C
ATOM    554  C   ASP A  71      28.969  48.474  -5.898  1.00 52.41 C
ATOM    555  O   ASP A  71      28.508  49.224  -6.764  1.00 47.41 O
ATOM    556  CB  ASP A  71      28.406  46.166  -6.708  1.00 49.99 C
ATOM    557  CG  ASP A  71      28.892  44.834  -7.302  1.00 49.02 C
ATOM    558  OD1 ASP A  71      29.813  44.825  -8.146  1.00 46.46 O
ATOM    559  OD2 ASP A  71      28.324  43.784  -6.929  1.00 50.74 O
ATOM    560  N   ALA A  72      28.987  48.801  -4.610  1.00 42.72 N
ATOM    561  CA  ALA A  72      28.429  50.063  -4.133  1.00 45.31 C
ATOM    562  C   ALA A  72      29.129  51.291  -4.686  1.00 47.73 C
ATOM    563  O   ALA A  72      30.326  51.268  -4.977  1.00 47.41 O
ATOM    564  CB  ALA A  72      28.460  50.107  -2.604  1.00 47.05 C
ATOM    565  N   GLY A  73      28.378  52.374  -4.821  1.00 48.72 N
ATOM    566  CA  GLY A  73      28.976  53.593  -5.322  1.00 54.09 C
ATOM    567  C   GLY A  73      28.144  54.331  -6.341  1.00 51.98 C
```

Figure 2 (Table 2 (page 18))

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ATOM    568  O   GLY A  73      27.018  53.939  -6.653  1.00 49.57 O
ATOM    569  N   ILE A  74      28.716  55.413  -6.859  1.00 51.79 N
ATOM    570  CA  ILE A  74      28.052  56.242  -7.850  1.00 48.58 C
ATOM    571  C   ILE A  74      28.428  55.760  -9.237  1.00 47.75 C
ATOM    572  O   ILE A  74      29.603  55.780  -9.620  1.00 46.87 O
ATOM    573  CB  ILE A  74      28.475  57.717  -7.705  1.00 54.10 C
ATOM    574  CG1 ILE A  74      28.061  58.227  -6.323  1.00 60.29 C
ATOM    575  CG2 ILE A  74      27.860  58.551  -8.816  1.00 51.72 C
ATOM    576  CD1 ILE A  74      28.463  59.656  -6.041  1.00 55.15 C
ATOM    577  N   TYR A  75      27.429  55.272  -9.960  1.00 39.87 N
ATOM    578  CA  TYR A  75      27.637  54.826 -11.330  1.00 48.23 C
ATOM    579  C   TYR A  75      27.168  56.010 -12.126  1.00 48.15 C
ATOM    580  O   TYR A  75      26.293  56.764 -11.682  1.00 46.43 O
ATOM    581  CB  TYR A  75      26.745  53.629 -11.707  1.00 44.56 C
ATOM    582  CG  TYR A  75      27.137  52.331 -11.050  1.00 47.56 C
ATOM    583  CD1 TYR A  75      26.925  52.133  -9.682  1.00 39.03 C
ATOM    584  CD2 TYR A  75      27.789  51.326 -11.773  1.00 43.44 C
ATOM    585  CE1 TYR A  75      27.356  50.967  -9.045  1.00 39.99 C
ATOM    586  CE2 TYR A  75      28.230  50.162 -11.146  1.00 32.79 C
ATOM    587  CZ  TYR A  75      28.010  49.990  -9.778  1.00 35.84 C
ATOM    588  OH  TYR A  75      28.463  48.851  -9.153  1.00 43.95 O
ATOM    589  N   LYS A  76      27.739  56.201 -13.299  1.00 48.85 N
ATOM    590  CA  LYS A  76      27.270  57.305 -14.090  1.00 48.84 C
ATOM    591  C   LYS A  76      27.178  56.938 -15.532  1.00 44.98 C
ATOM    592  O   LYS A  76      27.912  56.092 -16.052  1.00 47.18 O
ATOM    593  CB  LYS A  76      28.115  58.551 -13.857  1.00 56.56 C
ATOM    594  CG  LYS A  76      29.442  58.619 -14.520  1.00 59.09 C
ATOM    595  CD  LYS A  76      30.046  59.941 -14.072  1.00 66.83 C
ATOM    596  CE  LYS A  76      31.142  60.452 -14.968  1.00 71.43 C
ATOM    597  NZ  LYS A  76      31.553  61.794 -14.449  1.00 73.15 N
ATOM    598  N   CYS A  77      26.194  57.553 -16.153  1.00 45.89 N
ATOM    599  CA  CYS A  77      25.888  57.319 -17.532  1.00 44.65 C
ATOM    600  C   CYS A  77      26.233  58.600 -18.270  1.00 47.89 C
ATOM    601  O   CYS A  77      25.718  59.666 -17.945  1.00 52.98 O
ATOM    602  CB  CYS A  77      24.401  57.004 -17.652  1.00 42.61 C
ATOM    603  SG  CYS A  77      23.808  56.802 -19.350  1.00 61.23 S
ATOM    604  N   VAL A  78      27.122  58.494 -19.249  1.00 50.12 N
ATOM    605  CA  VAL A  78      27.547  59.658 -20.019  1.00 46.50 C
ATOM    606  C   VAL A  78      27.082  59.581 -21.471  1.00 43.99 C
ATOM    607  O   VAL A  78      27.222  58.552 -22.131  1.00 48.45 O
ATOM    608  CB  VAL A  78      29.084  59.795 -19.993  1.00 46.58 C
ATOM    609  CG1 VAL A  78      29.517  61.010 -20.820  1.00 51.99 C
ATOM    610  CG2 VAL A  78      29.566  59.942 -18.547  1.00 41.06 C
ATOM    611  N   VAL A  79      26.521  60.672 -21.965  1.00 48.68 N
ATOM    612  CA  VAL A  79      26.047  60.720 -23.343  1.00 57.39 C
ATOM    613  C   VAL A  79      26.945  61.666 -24.119  1.00 54.87 C
ATOM    614  O   VAL A  79      27.194  62.792 -23.691  1.00 52.91 O
ATOM    615  CB  VAL A  79      24.598  61.227 -23.417  1.00 60.20 C
ATOM    616  CG1 VAL A  79      24.085  61.155 -24.848  1.00 54.06 C
ATOM    617  CG2 VAL A  79      23.730  60.395 -22.487  1.00 56.02 C
ATOM    618  N   THR A  80      27.452  61.191 -25.247  1.00 48.32 N
ATOM    619  CA  THR A  80      28.313  62.011 -26.066  1.00 52.81 C
ATOM    620  C   THR A  80      27.706  62.226 -27.450  1.00 54.17 C
ATOM    621  O   THR A  80      27.501  61.266 -28.187  1.00 49.22 O
ATOM    622  CB  THR A  80      29.691  61.371 -26.241  1.00 54.94 C
ATOM    623  OG1 THR A  80      30.268  61.104 -24.954  1.00 54.31 O
ATOM    624  CG2 THR A  80      30.601  62.318 -27.012  1.00 41.33 C
```

Figure 2 (Table 2 (page 19))

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ATOM    625  N   ALA A  81      27.430  63.487 -27.787  1.00 56.76 N
ATOM    626  CA  ALA A  81      26.859  63.866 -29.088  1.00 58.85 C
ATOM    627  C   ALA A  81      27.942  63.828 -30.165  1.00 58.97 C
ATOM    628  O   ALA A  81      29.131  63.922 -29.847  1.00 53.72 O
ATOM    629  CB  ALA A  81      26.263  65.265 -29.005  1.00 60.88 C
ATOM    630  N   GLU A  82      27.528  63.712 -31.429  1.00 67.86 N
ATOM    631  CA  GLU A  82      28.462  63.639 -32.555  1.00 73.18 C
ATOM    632  C   GLU A  82      29.599  64.664 -32.507  1.00 68.06 C
ATOM    633  O   GLU A  82      30.700  64.398 -32.993  1.00 65.36 O
ATOM    634  CB  GLU A  82      27.707  63.768 -33.887  1.00 74.95 C
ATOM    635  CG  GLU A  82      28.027  62.638 -34.868  1.00 98.35 C
ATOM    636  CD  GLU A  82      27.295  62.768 -36.194  1.00111.66 C
ATOM    637  OE1 GLU A  82      26.071  63.034 -36.178  1.00118.11 O
ATOM    638  OE2 GLU A  82      27.942  62.594 -37.253  1.00117.01 O
ATOM    639  N   ASP A  83      29.340  65.821 -31.907  1.00 62.35 N
ATOM    640  CA  ASP A  83      30.340  66.877 -31.812  1.00 67.89 C
ATOM    641  C   ASP A  83      31.171  66.830 -30.533  1.00 71.00 C
ATOM    642  O   ASP A  83      31.929  67.759 -30.246  1.00 73.73 O
ATOM    643  CB  ASP A  83      29.653  68.230 -31.924  1.00 74.31 C
ATOM    644  CG  ASP A  83      28.664  68.461 -30.815  1.00 82.18 C
ATOM    645  OD1 ASP A  83      27.939  67.508 -30.462  1.00 93.75 O
ATOM    646  OD2 ASP A  83      28.606  69.593 -30.301  1.00 87.77 O
ATOM    647  N   GLY A  84      31.017  65.760 -29.759  1.00 69.26 N
ATOM    648  CA  GLY A  84      31.790  65.617 -28.533  1.00 61.95 C
ATOM    649  C   GLY A  84      31.242  66.254 -27.266  1.00 62.86 C
ATOM    650  O   GLY A  84      31.851  66.139 -26.197  1.00 65.82 O
ATOM    651  N   THR A  85      30.106  66.936 -27.361  1.00 55.77 N
ATOM    652  CA  THR A  85      29.535  67.559 -26.176  1.00 63.65 C
ATOM    653  C   THR A  85      28.929  66.445 -25.320  1.00 61.95 C
ATOM    654  O   THR A  85      28.291  65.528 -25.839  1.00 56.86 O
ATOM    655  CB  THR A  85      28.471  68.614 -26.555  1.00 61.72 C
ATOM    656  OG1 THR A  85      27.458  68.019 -27.373  1.00 73.83 O
ATOM    657  CG2 THR A  85      29.125  69.749 -27.325  1.00 69.89 C
ATOM    658  N   GLN A  86      29.130  66.520 -24.011  1.00 58.16 N
ATOM    659  CA  GLN A  86      28.628  65.464 -23.141  1.00 63.76 C
ATOM    660  C   GLN A  86      27.696  65.900 -22.030  1.00 62.47 C
ATOM    661  O   GLN A  86      27.803  67.011 -21.505  1.00 64.92 O
ATOM    662  CB  GLN A  86      29.793  64.715 -22.498  1.00 56.96 C
ATOM    663  CG  GLN A  86      30.860  64.242 -23.460  1.00 50.20 C
ATOM    664  CD  GLN A  86      31.964  63.519 -22.724  1.00 54.10 C
ATOM    665  OE1 GLN A  86      32.390  63.965 -21.663  1.00 54.08 O
ATOM    666  NE2 GLN A  86      32.436  62.401 -23.276  1.00 56.27 N
ATOM    667  N   SER A  87      26.800  64.986 -21.667  1.00 63.47 N
ATOM    668  CA  SER A  87      25.836  65.182 -20.588  1.00 68.11 C
ATOM    669  C   SER A  87      25.889  63.906 -19.749  1.00 65.62 C
ATOM    670  O   SER A  87      26.194  62.829 -20.270  1.00 69.37 O
ATOM    671  CB  SER A  87      24.420  65.362 -21.150  1.00 75.52 C
ATOM    672  OG  SER A  87      24.344  66.449 -22.057  1.00 88.36 O
ATOM    673  N   GLU A  88      25.592  64.009 -18.460  1.00 63.19 N
ATOM    674  CA  GLU A  88      25.623  62.827 -17.607  1.00 53.44 C
ATOM    675  C   GLU A  88      24.532  62.803 -16.556  1.00 59.13 C
ATOM    676  O   GLU A  88      23.942  63.824 -16.209  1.00 58.88 O
ATOM    677  CB  GLU A  88      26.976  62.711 -16.904  1.00 60.59 C
ATOM    678  CG  GLU A  88      27.272  63.816 -15.898  1.00 67.25 C
ATOM    679  CD  GLU A  88      28.656  63.687 -15.277  1.00 78.40 C
ATOM    680  OE1 GLU A  88      29.631  63.494 -16.035  1.00 79.36 O
ATOM    681  OE2 GLU A  88      28.773  63.782 -14.033  1.00 81.96 O
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Figure 2 (Table 2 (page 20))

ATOM	682	N	ALA	A	89	24.254	61.602	-16.079	1.00	54.88	N
ATOM	683	CA	ALA	A	89	23.283	61.384	-15.027	1.00	45.50	C
ATOM	684	C	ALA	A	89	24.036	60.407	-14.149	1.00	52.74	C
ATOM	685	O	ALA	A	89	24.777	59.552	-14.659	1.00	48.26	O
ATOM	686	CB	ALA	A	89	22.022	60.736	-15.567	1.00	53.66	C
ATOM	687	N	THR	A	90	23.887	60.549	-12.839	1.00	46.21	N
ATOM	688	CA	THR	A	90	24.558	59.647	-11.932	1.00	49.08	C
ATOM	689	C	THR	A	90	23.515	58.993	-11.051	1.00	49.13	C
ATOM	690	O	THR	A	90	22.402	59.516	-10.861	1.00	49.24	O
ATOM	691	CB	THR	A	90	25.587	60.376	-11.052	1.00	48.30	C
ATOM	692	OG1	THR	A	90	24.932	61.366	-10.256	1.00	53.97	O
ATOM	693	CG2	THR	A	90	26.640	61.041	-11.915	1.00	52.65	C
ATOM	694	N	VAL	A	91	23.871	57.823	-10.539	1.00	45.14	N
ATOM	695	CA	VAL	A	91	22.966	57.102	-9.667	1.00	48.65	C
ATOM	696	C	VAL	A	91	23.736	56.474	-8.527	1.00	45.53	C
ATOM	697	O	VAL	A	91	24.708	55.754	-8.740	1.00	47.93	O
ATOM	698	CB	VAL	A	91	22.164	56.035	-10.433	1.00	50.62	C
ATOM	699	CG1	VAL	A	91	23.113	55.013	-11.094	1.00	48.35	C
ATOM	700	CG2	VAL	A	91	21.177	55.349	-9.474	1.00	54.01	C
ATOM	701	N	ASN	A	92	23.304	56.773	-7.306	1.00	49.96	N
ATOM	702	CA	ASN	A	92	23.964	56.255	-6.116	1.00	50.90	C
ATOM	703	C	ASN	A	92	23.399	54.887	-5.780	1.00	45.05	C
ATOM	704	O	ASN	A	92	22.220	54.742	-5.466	1.00	48.81	O
ATOM	705	CB	ASN	A	92	23.757	57.200	-4.932	1.00	47.93	C
ATOM	706	CG	ASN	A	92	24.569	56.786	-3.724	1.00	54.25	C
ATOM	707	OD1	ASN	A	92	24.115	56.897	-2.584	1.00	56.44	O
ATOM	708	ND2	ASN	A	92	25.784	56.304	-3.969	1.00	54.09	N
ATOM	709	N	VAL	A	93	24.256	53.881	-5.851	1.00	46.44	N
ATOM	710	CA	VAL	A	93	23.831	52.527	-5.574	1.00	47.68	C
ATOM	711	C	VAL	A	93	24.387	52.085	-4.232	1.00	46.87	C
ATOM	712	O	VAL	A	93	25.602	52.009	-4.053	1.00	45.39	O
ATOM	713	CB	VAL	A	93	24.310	51.548	-6.679	1.00	44.88	C
ATOM	714	CG1	VAL	A	93	23.834	50.143	-6.365	1.00	50.34	C
ATOM	715	CG2	VAL	A	93	23.769	51.981	-8.042	1.00	51.13	C
ATOM	716	N	LYS	A	94	23.490	51.807	-3.290	1.00	52.11	N
ATOM	717	CA	LYS	A	94	23.902	51.347	-1.961	1.00	59.43	C
ATOM	718	C	LYS	A	94	23.774	49.832	-1.886	1.00	55.63	C
ATOM	719	O	LYS	A	94	22.871	49.241	-2.471	1.00	43.24	O
ATOM	720	CB	LYS	A	94	23.033	51.960	-0.855	1.00	55.35	C
ATOM	721	CG	LYS	A	94	23.173	53.464	-0.668	1.00	65.17	C
ATOM	722	CD	LYS	A	94	22.156	53.977	0.356	1.00	67.48	C
ATOM	723	CE	LYS	A	94	22.081	55.492	0.362	1.00	74.84	C
ATOM	724	NZ	LYS	A	94	21.040	55.986	1.310	1.00	78.54	N
ATOM	725	N	ILE	A	95	24.699	49.202	-1.181	1.00	56.66	N
ATOM	726	CA	ILE	A	95	24.658	47.762	-1.004	1.00	56.71	C
ATOM	727	C	ILE	A	95	24.467	47.546	0.495	1.00	59.65	C
ATOM	728	O	ILE	A	95	25.004	48.298	1.305	1.00	53.96	O
ATOM	729	CB	ILE	A	95	25.981	47.086	-1.451	1.00	50.11	C
ATOM	730	CG1	ILE	A	95	26.247	47.361	-2.935	1.00	58.21	C
ATOM	731	CG2	ILE	A	95	25.905	45.584	-1.206	1.00	55.81	C
ATOM	732	CD1	ILE	A	95	25.141	46.878	-3.869	1.00	46.59	C
ATOM	733	N	PHE	A	96	23.670	46.553	0.863	1.00	56.77	N
ATOM	734	CA	PHE	A	96	23.464	46.249	2.269	1.00	56.57	C
ATOM	735	C	PHE	A	96	23.070	44.791	2.380	1.00	52.33	C
ATOM	736	O	PHE	A	96	22.921	44.087	1.375	1.00	55.58	O
ATOM	737	CB	PHE	A	96	22.389	47.146	2.893	1.00	51.68	C

Figure 2 (Table 2 (page 21))

ATOM	738	CG	PHE	A	96	20.984	46.731	2.570	1.00	55.80	C
ATOM	739	CD1	PHE	A	96	20.078	46.441	3.589	1.00	56.18	C
ATOM	740	CD2	PHE	A	96	20.565	46.630	1.249	1.00	53.68	C
ATOM	741	CE1	PHE	A	96	18.770	46.055	3.287	1.00	61.36	C
ATOM	742	CE2	PHE	A	96	19.268	46.249	0.932	1.00	54.41	C
ATOM	743	CZ	PHE	A	96	18.362	45.959	1.951	1.00	51.56	C
ATOM	744	N	GLN	A	97	22.929	44.323	3.607	1.00	44.80	N
ATOM	745	CA	GLN	A	97	22.565	42.945	3.819	1.00	41.35	C
ATOM	746	C	GLN	A	97	21.257	42.956	4.559	1.00	43.49	C
ATOM	747	O	GLN	A	97	21.185	43.352	5.725	1.00	48.61	O
ATOM	748	CB	GLN	A	97	23.639	42.220	4.639	1.00	50.03	C
ATOM	749	CG	GLN	A	97	23.239	40.811	5.074	1.00	42.38	C
ATOM	750	CD	GLN	A	97	22.968	39.885	3.899	1.00	45.87	C
ATOM	751	OE1	GLN	A	97	23.879	39.539	3.148	1.00	50.97	O
ATOM	752	NE2	GLN	A	97	21.712	39.485	3.725	1.00	43.50	N
ATOM	753	N	LYS	A	98	20.208	42.557	3.861	1.00	43.56	N
ATOM	754	CA	LYS	A	98	18.914	42.503	4.493	1.00	50.07	C
ATOM	755	C	LYS	A	98	18.988	41.436	5.594	1.00	45.12	C
ATOM	756	O	LYS	A	98	19.772	40.483	5.518	1.00	44.19	O
ATOM	757	CB	LYS	A	98	17.835	42.141	3.467	1.00	42.89	C
ATOM	758	CG	LYS	A	98	17.806	40.689	3.029	1.00	54.06	C
ATOM	759	CD	LYS	A	98	16.620	40.432	2.091	1.00	70.03	C
ATOM	760	CE	LYS	A	98	16.542	38.972	1.674	1.00	74.47	C
ATOM	761	NZ	LYS	A	98	15.366	38.722	0.799	1.00	87.06	N
ATOM	762	N	LEU	A	99	18.187	41.633	6.625	1.00	42.33	N
ATOM	763	CA	LEU	A	99	18.112	40.718	7.743	1.00	48.11	C
ATOM	764	C	LEU	A	99	17.731	39.322	7.271	1.00	51.43	C
ATOM	765	O	LEU	A	99	16.622	39.119	6.784	1.00	54.69	O
ATOM	766	CB	LEU	A	99	17.058	41.223	8.727	1.00	40.97	C
ATOM	767	CG	LEU	A	99	16.874	40.365	9.974	1.00	51.52	C
ATOM	768	CD1	LEU	A	99	18.114	40.494	10.829	1.00	49.68	C
ATOM	769	CD2	LEU	A	99	15.663	40.822	10.765	1.00	51.15	C
ATOM	770	N	MET	A	100	18.643	38.358	7.388	1.00	48.12	N
ATOM	771	CA	MET	A	100	18.321	36.984	6.995	1.00	51.56	C
ATOM	772	C	MET	A	100	19.033	35.977	7.907	1.00	51.77	C
ATOM	773	O	MET	A	100	19.991	36.322	8.621	1.00	39.76	O
ATOM	774	CB	MET	A	100	18.650	36.727	5.512	1.00	61.21	C
ATOM	775	CG	MET	A	100	20.116	36.564	5.166	1.00	69.49	C
ATOM	776	SD	MET	A	100	20.416	36.505	3.372	1.00	84.60	S
ATOM	777	CE	MET	A	100	19.818	34.884	2.949	1.00	92.44	C
ATOM	778	N	PHE	A	101	18.531	34.745	7.908	1.00	45.49	N
ATOM	779	CA	PHE	A	101	19.085	33.684	8.732	1.00	50.26	C
ATOM	780	C	PHE	A	101	20.138	32.893	7.995	1.00	43.40	C
ATOM	781	O	PHE	A	101	19.907	32.400	6.902	1.00	61.65	O
ATOM	782	CB	PHE	A	101	17.969	32.769	9.210	1.00	46.80	C
ATOM	783	CG	PHE	A	101	17.019	33.450	10.137	1.00	46.54	C
ATOM	784	CD1	PHE	A	101	15.900	34.112	9.652	1.00	52.32	C
ATOM	785	CD2	PHE	A	101	17.274	33.488	11.499	1.00	44.46	C
ATOM	786	CE1	PHE	A	101	15.054	34.822	10.516	1.00	43.20	C
ATOM	787	CE2	PHE	A	101	16.441	34.192	12.366	1.00	48.20	C
ATOM	788	CZ	PHE	A	101	15.322	34.858	11.869	1.00	48.40	C
ATOM	789	N	LYS	A	102	21.302	32.771	8.611	1.00	51.46	N
ATOM	790	CA	LYS	A	102	22.420	32.066	8.009	1.00	48.23	C
ATOM	791	C	LYS	A	102	22.516	30.619	8.468	1.00	54.86	C
ATOM	792	O	LYS	A	102	22.768	29.712	7.668	1.00	62.07	O
ATOM	793	CB	LYS	A	102	23.714	32.799	8.340	1.00	57.97	C

Figure 2 (Table 2 (page 22))

ATOM	794	CG	LYS	A	102	24.954	32.199	7.720	1.00	71.82 C
ATOM	795	CD	LYS	A	102	26.170	33.021	8.108	1.00	82.19 C
ATOM	796	CE	LYS	A	102	27.335	32.773	7.169	1.00	88.42 C
ATOM	797	NZ	LYS	A	102	28.516	33.602	7.540	1.00	98.10 N
ATOM	798	N	ASN	A	103	22.328	30.409	9.763	1.00	47.83 N
ATOM	799	CA	ASN	A	103	22.379	29.081	10.339	1.00	43.78 C
ATOM	800	C	ASN	A	103	21.419	29.084	11.525	1.00	45.04 C
ATOM	801	O	ASN	A	103	21.661	29.751	12.534	1.00	40.24 O
ATOM	802	CB	ASN	A	103	23.802	28.764	10.800	1.00	45.29 C
ATOM	803	CG	ASN	A	103	23.886	27.468	11.565	1.00	46.73 C
ATOM	804	OD1	ASN	A	103	23.582	26.402	11.037	1.00	54.61 O
ATOM	805	ND2	ASN	A	103	24.308	27.552	12.822	1.00	50.10 N
ATOM	806	N	ALA	A	104	20.312	28.369	11.379	1.00	40.89 N
ATOM	807	CA	ALA	A	104	19.304	28.264	12.422	1.00	48.41 C
ATOM	808	C	ALA	A	104	18.651	26.906	12.200	1.00	52.07 C
ATOM	809	O	ALA	A	104	17.490	26.811	11.829	1.00	51.94 O
ATOM	810	CB	ALA	A	104	18.280	29.359	12.241	1.00	53.18 C
ATOM	811	N	PRO	A	105	19.386	25.834	12.461	1.00	47.52 N
ATOM	812	CA	PRO	A	105	18.873	24.481	12.265	1.00	45.57 C
ATOM	813	C	PRO	A	105	17.700	24.096	13.112	1.00	47.49 C
ATOM	814	O	PRO	A	105	17.508	24.606	14.223	1.00	41.72 O
ATOM	815	CB	PRO	A	105	20.087	23.588	12.501	1.00	49.47 C
ATOM	816	CG	PRO	A	105	21.055	24.460	13.270	1.00	52.18 C
ATOM	817	CD	PRO	A	105	20.631	25.867	13.230	1.00	52.90 C
ATOM	818	N	THR	A	106	16.864	23.260	12.515	1.00	48.69 N
ATOM	819	CA	THR	A	106	15.717	22.758	13.215	1.00	52.32 C
ATOM	820	C	THR	A	106	15.529	21.322	12.759	1.00	58.90 C
ATOM	821	O	THR	A	106	15.672	20.999	11.581	1.00	55.09 O
ATOM	822	CB	THR	A	106	14.447	23.612	12.955	1.00	53.67 C
ATOM	823	OG1	THR	A	106	13.355	23.053	13.698	1.00	54.59 O
ATOM	824	CG2	THR	A	106	14.097	23.641	11.468	1.00	58.16 C
ATOM	825	N	PRO	A	107	15.275	20.424	13.714	1.00	52.16 N
ATOM	826	CA	PRO	A	107	15.184	20.737	15.138	1.00	43.22 C
ATOM	827	C	PRO	A	107	16.585	20.810	15.732	1.00	47.05 C
ATOM	828	O	PRO	A	107	17.578	20.532	15.064	1.00	45.59 O
ATOM	829	CB	PRO	A	107	14.426	19.539	15.688	1.00	49.39 C
ATOM	830	CG	PRO	A	107	15.052	18.411	14.902	1.00	55.45 C
ATOM	831	CD	PRO	A	107	15.065	18.986	13.480	1.00	55.64 C
ATOM	832	N	GLN	A	108	16.650	21.202	16.994	1.00	40.58 N
ATOM	833	CA	GLN	A	108	17.901	21.229	17.709	1.00	46.97 C
ATOM	834	C	GLN	A	108	17.566	20.339	18.896	1.00	44.47 C
ATOM	835	O	GLN	A	108	16.492	20.467	19.489	1.00	36.69 O
ATOM	836	CB	GLN	A	108	18.271	22.657	18.084	1.00	40.68 C
ATOM	837	CG	GLN	A	108	18.770	23.436	16.846	1.00	37.05 C
ATOM	838	CD	GLN	A	108	19.203	24.847	17.171	1.00	40.43 C
ATOM	839	OE1	GLN	A	108	19.879	25.073	18.172	1.00	36.29 O
ATOM	840	NE2	GLN	A	108	18.828	25.805	16.332	1.00	37.82 N
ATOM	841	N	GLU	A	109	18.469	19.413	19.203	1.00	38.32 N
ATOM	842	CA	GLU	A	109	18.261	18.425	20.257	1.00	39.59 C
ATOM	843	C	GLU	A	109	19.216	18.551	21.424	1.00	44.20 C
ATOM	844	O	GLU	A	109	20.380	18.922	21.254	1.00	41.88 O
ATOM	845	CB	GLU	A	109	18.364	17.033	19.637	1.00	39.87 C
ATOM	846	CG	GLU	A	109	17.437	16.885	18.448	1.00	45.54 C
ATOM	847	CD	GLU	A	109	17.358	15.478	17.912	1.00	49.95 C
ATOM	848	OE1	GLU	A	109	17.335	14.518	18.713	1.00	54.48 O
ATOM	849	OE2	GLU	A	109	17.295	15.330	16.678	1.00	54.37 O

Figure 2 (Table 2 (page 23))

ATOM	850	N	PHE	A	110	18.713	18.223	22.609	1.00	36.31	N
ATOM	851	CA	PHE	A	110	19.491	18.314	23.825	1.00	37.31	C
ATOM	852	C	PHE	A	110	19.154	17.167	24.748	1.00	44.15	C
ATOM	853	O	PHE	A	110	18.071	16.596	24.694	1.00	42.74	O
ATOM	854	CB	PHE	A	110	19.202	19.643	24.531	1.00	29.73	C
ATOM	855	CG	PHE	A	110	19.299	20.831	23.612	1.00	36.45	C
ATOM	856	CD1	PHE	A	110	18.189	21.286	22.922	1.00	37.59	C
ATOM	857	CD2	PHE	A	110	20.522	21.445	23.387	1.00	35.71	C
ATOM	858	CE1	PHE	A	110	18.301	22.337	22.006	1.00	49.86	C
ATOM	859	CE2	PHE	A	110	20.649	22.489	22.476	1.00	43.61	C
ATOM	860	CZ	PHE	A	110	19.533	22.939	21.785	1.00	39.36	C
ATOM	861	N	LYS	A	111	20.108	16.819	25.592	1.00	38.44	N
ATOM	862	CA	LYS	A	111	19.909	15.745	26.533	1.00	39.53	C
ATOM	863	C	LYS	A	111	19.327	16.395	27.769	1.00	33.66	C
ATOM	864	O	LYS	A	111	19.832	17.419	28.238	1.00	37.40	O
ATOM	865	CB	LYS	A	111	21.254	15.075	26.845	1.00	35.52	C
ATOM	866	CG	LYS	A	111	21.185	13.974	27.890	1.00	45.41	C
ATOM	867	CD	LYS	A	111	22.548	13.272	28.006	1.00	51.44	C
ATOM	868	CE	LYS	A	111	22.515	12.114	29.000	1.00	58.54	C
ATOM	869	NZ	LYS	A	111	23.657	11.172	28.765	1.00	62.26	N
ATOM	870	N	GLU	A	112	18.255	15.810	28.287	1.00	39.60	N
ATOM	871	CA	GLU	A	112	17.614	16.339	29.478	1.00	42.51	C
ATOM	872	C	GLU	A	112	18.627	16.706	30.569	1.00	37.78	C
ATOM	873	O	GLU	A	112	19.554	15.950	30.846	1.00	41.69	O
ATOM	874	CB	GLU	A	112	16.621	15.312	30.034	1.00	42.05	C
ATOM	875	CG	GLU	A	112	15.743	15.888	31.120	1.00	48.02	C
ATOM	876	CD	GLU	A	112	14.735	14.886	31.675	1.00	67.88	C
ATOM	877	OE1	GLU	A	112	13.582	15.304	31.937	1.00	64.90	O
ATOM	878	OE2	GLU	A	112	15.093	13.700	31.865	1.00	70.27	O
ATOM	879	N	GLY	A	113	18.448	17.875	31.175	1.00	41.71	N
ATOM	880	CA	GLY	A	113	19.350	18.298	32.228	1.00	43.96	C
ATOM	881	C	GLY	A	113	20.555	19.128	31.824	1.00	46.88	C
ATOM	882	O	GLY	A	113	21.087	19.877	32.652	1.00	44.90	O
ATOM	883	N	GLU	A	114	21.017	19.021	30.584	1.00	41.27	N
ATOM	884	CA	GLU	A	114	22.181	19.830	30.227	1.00	49.33	C
ATOM	885	C	GLU	A	114	21.739	21.260	29.927	1.00	46.85	C
ATOM	886	O	GLU	A	114	20.539	21.551	29.864	1.00	45.47	O
ATOM	887	CB	GLU	A	114	22.957	19.199	29.052	1.00	46.70	C
ATOM	888	CG	GLU	A	114	22.319	19.293	27.682	1.00	49.46	C
ATOM	889	CD	GLU	A	114	23.076	18.490	26.613	1.00	56.05	C
ATOM	890	OE1	GLU	A	114	24.174	17.946	26.894	1.00	59.22	O
ATOM	891	OE2	GLU	A	114	22.565	18.407	25.482	1.00	51.60	O
ATOM	892	N	ASP	A	115	22.689	22.181	29.822	1.00	42.06	N
ATOM	893	CA	ASP	A	115	22.323	23.554	29.512	1.00	46.33	C
ATOM	894	C	ASP	A	115	22.184	23.568	28.018	1.00	46.24	C
ATOM	895	O	ASP	A	115	23.107	23.195	27.299	1.00	51.16	O
ATOM	896	CB	ASP	A	115	23.394	24.525	29.976	1.00	52.16	C
ATOM	897	CG	ASP	A	115	23.530	24.535	31.475	1.00	58.98	C
ATOM	898	OD1	ASP	A	115	22.515	24.291	32.169	1.00	56.34	O
ATOM	899	OD2	ASP	A	115	24.647	24.785	31.959	1.00	74.61	O
ATOM	900	N	ALA	A	116	21.009	23.943	27.536	1.00	40.21	N
ATOM	901	CA	ALA	A	116	20.812	23.937	26.105	1.00	41.98	C
ATOM	902	C	ALA	A	116	21.024	25.315	25.524	1.00	39.57	C
ATOM	903	O	ALA	A	116	20.591	26.311	26.093	1.00	41.84	O
ATOM	904	CB	ALA	A	116	19.406	23.428	25.761	1.00	37.59	C
ATOM	905	N	VAL	A	117	21.711	25.374	24.396	1.00	35.34	N

Figure 2 (Table 2 (page 24))

```
ATOM    906  CA  VAL A 117      21.907  26.651  23.736  1.00 34.85 C
ATOM    907  C   VAL A 117      21.305  26.459  22.356  1.00 34.14 C
ATOM    908  O   VAL A 117      21.751  25.608  21.603  1.00 35.50 O
ATOM    909  CB  VAL A 117      23.391  26.997  23.612  1.00 40.36 C
ATOM    910  CG1 VAL A 117      23.573  28.240  22.764  1.00 35.45 C
ATOM    911  CG2 VAL A 117      23.957  27.265  24.994  1.00 46.40 C
ATOM    912  N   ILE A 118      20.276  27.244  22.046  1.00 35.04 N
ATOM    913  CA  ILE A 118      19.593  27.169  20.757  1.00 34.21 C
ATOM    914  C   ILE A 118      20.257  28.172  19.836  1.00 25.24 C
ATOM    915  O   ILE A 118      20.252  29.371  20.095  1.00 32.78 O
ATOM    916  CB  ILE A 118      18.106  27.535  20.901  1.00 34.79 C
ATOM    917  CG1 ILE A 118      17.471  26.651  21.978  1.00 43.37 C
ATOM    918  CG2 ILE A 118      17.384  27.289  19.578  1.00 35.72 C
ATOM    919  CD1 ILE A 118      16.071  27.043  22.340  1.00 58.55 C
ATOM    920  N   VAL A 119      20.829  27.649  18.771  1.00 31.01 N
ATOM    921  CA  VAL A 119      21.593  28.441  17.830  1.00 37.30 C
ATOM    922  C   VAL A 119      20.771  29.119  16.753  1.00 37.56 C
ATOM    923  O   VAL A 119      19.983  28.491  16.065  1.00 40.50 O
ATOM    924  CB  VAL A 119      22.670  27.549  17.175  1.00 35.82 C
ATOM    925  CG1 VAL A 119      23.467  28.340  16.136  1.00 34.06 C
ATOM    926  CG2 VAL A 119      23.582  27.004  18.258  1.00 34.59 C
ATOM    927  N   CYS A 120      20.980  30.414  16.620  1.00 36.81 N
ATOM    928  CA  CYS A 120      20.286  31.194  15.610  1.00 32.12 C
ATOM    929  C   CYS A 120      21.262  32.279  15.148  1.00 33.42 C
ATOM    930  O   CYS A 120      21.534  33.244  15.873  1.00 34.81 O
ATOM    931  CB  CYS A 120      19.027  31.819  16.211  1.00 41.13 C
ATOM    932  SG  CYS A 120      17.972  32.754  15.028  1.00 50.41 S
ATOM    933  N   ASP A 121      21.821  32.082  13.959  1.00 36.26 N
ATOM    934  CA  ASP A 121      22.778  33.020  13.370  1.00 38.88 C
ATOM    935  C   ASP A 121      22.109  33.906  12.333  1.00 36.35 C
ATOM    936  O   ASP A 121      21.607  33.429  11.326  1.00 41.43 O
ATOM    937  CB  ASP A 121      23.934  32.251  12.720  1.00 41.76 C
ATOM    938  CG  ASP A 121      24.766  31.509  13.744  1.00 40.59 C
ATOM    939  OD1 ASP A 121      25.129  32.153  14.749  1.00 47.54 O
ATOM    940  OD2 ASP A 121      25.047  30.306  13.560  1.00 45.40 O
ATOM    941  N   VAL A 122      22.099  35.202  12.584  1.00 41.75 N
ATOM    942  CA  VAL A 122      21.495  36.119  11.636  1.00 52.79 C
ATOM    943  C   VAL A 122      22.563  36.999  11.025  1.00 52.22 C
ATOM    944  O   VAL A 122      23.670  37.115  11.550  1.00 45.91 O
ATOM    945  CB  VAL A 122      20.458  37.052  12.302  1.00 53.37 C
ATOM    946  CG1 VAL A 122      19.391  36.242  12.998  1.00 50.48 C
ATOM    947  CG2 VAL A 122      21.153  37.986  13.275  1.00 58.84 C
ATOM    948  N   VAL A 123      22.215  37.609   9.901  1.00 47.92 N
ATOM    949  CA  VAL A 123      23.104  38.525   9.211  1.00 44.45 C
ATOM    950  C   VAL A 123      22.279  39.739   8.809  1.00 53.24 C
ATOM    951  O   VAL A 123      21.097  39.610   8.449  1.00 44.25 O
ATOM    952  CB  VAL A 123      23.713  37.910   7.941  1.00 53.12 C
ATOM    953  CG1 VAL A 123      24.633  36.758   8.307  1.00 58.99 C
ATOM    954  CG2 VAL A 123      22.610  37.442   7.012  1.00 54.51 C
ATOM    955  N   SER A 124      22.911  40.906   8.893  1.00 38.99 N
ATOM    956  CA  SER A 124      22.304  42.181   8.537  1.00 42.72 C
ATOM    957  C   SER A 124      23.383  43.252   8.618  1.00 46.36 C
ATOM    958  O   SER A 124      24.311  43.139   9.420  1.00 48.23 O
ATOM    959  CB  SER A 124      21.169  42.533   9.496  1.00 45.26 C
ATOM    960  OG  SER A 124      21.642  42.618  10.828  1.00 50.88 O
ATOM    961  N   SER A 125      23.257  44.283   7.787  1.00 48.24 N
```

Figure 2 (Table 2 (page 25))

ATOM	962	CA	SER	A	125	24.221	45.387	7.755	1.00	54.08 C
ATOM	963	C	SER	A	125	24.173	46.098	9.081	1.00	53.53 C
ATOM	964	O	SER	A	125	25.201	46.357	9.694	1.00	54.81 O
ATOM	965	CB	SER	A	125	23.874	46.373	6.641	1.00	45.61 C
ATOM	966	OG	SER	A	125	23.901	45.724	5.391	1.00	46.33 O
ATOM	967	N	LEU	A	126	22.961	46.408	9.519	1.00	51.93 N
ATOM	968	CA	LEU	A	126	22.756	47.077	10.795	1.00	60.20 C
ATOM	969	C	LEU	A	126	22.575	46.030	11.889	1.00	63.51 C
ATOM	970	O	LEU	A	126	22.012	44.961	11.657	1.00	63.28 O
ATOM	971	CB	LEU	A	126	21.521	47.987	10.726	1.00	67.31 C
ATOM	972	CG	LEU	A	126	21.606	49.171	9.746	1.00	75.52 C
ATOM	973	CD1	LEU	A	126	20.323	49.998	9.750	1.00	66.85 C
ATOM	974	CD2	LEU	A	126	22.791	50.045	10.141	1.00	72.14 C
ATOM	975	N	PRO	A	127	23.071	46.308	13.096	1.00	69.25 N
ATOM	976	CA	PRO	A	127	22.925	45.331	14.185	1.00	64.19 C
ATOM	977	C	PRO	A	127	21.463	45.007	14.524	1.00	57.99 C
ATOM	978	O	PRO	A	127	20.655	45.913	14.728	1.00	62.20 O
ATOM	979	CB	PRO	A	127	23.701	45.950	15.354	1.00	64.92 C
ATOM	980	CG	PRO	A	127	23.957	47.367	14.952	1.00	66.17 C
ATOM	981	CD	PRO	A	127	23.849	47.492	13.478	1.00	65.55 C
ATOM	982	N	PRO	A	128	21.126	43.698	14.610	1.00	61.71 N
ATOM	983	CA	PRO	A	128	19.782	43.195	14.906	1.00	61.85 C
ATOM	984	C	PRO	A	128	19.470	43.143	16.362	1.00	62.11 C
ATOM	985	O	PRO	A	128	20.351	42.980	17.192	1.00	64.26 O
ATOM	986	CB	PRO	A	128	19.805	41.776	14.340	1.00	58.63 C
ATOM	987	CG	PRO	A	128	21.070	41.714	13.493	1.00	66.61 C
ATOM	988	CD	PRO	A	128	22.009	42.561	14.287	1.00	51.57 C
ATOM	989	N	THR	A	129	18.196	43.270	16.669	1.00	56.05 N
ATOM	990	CA	THR	A	129	17.759	43.128	18.039	1.00	50.88 C
ATOM	991	C	THR	A	129	17.038	41.791	17.944	1.00	47.70 C
ATOM	992	O	THR	A	129	16.192	41.597	17.072	1.00	52.86 O
ATOM	993	CB	THR	A	129	16.801	44.243	18.457	1.00	59.29 C
ATOM	994	OG1	THR	A	129	17.564	45.360	18.933	1.00	64.98 O
ATOM	995	CG2	THR	A	129	15.885	43.769	19.562	1.00	68.98 C
ATOM	996	N	ILE	A	130	17.377	40.868	18.827	1.00	47.42 N
ATOM	997	CA	ILE	A	130	16.793	39.543	18.779	1.00	49.45 C
ATOM	998	C	ILE	A	130	15.829	39.251	19.914	1.00	48.06 C
ATOM	999	O	ILE	A	130	16.119	39.539	21.074	1.00	49.48 O
ATOM	1000	CB	ILE	A	130	17.907	38.480	18.805	1.00	52.16 C
ATOM	1001	CG1	ILE	A	130	18.711	38.558	17.510	1.00	55.93 C
ATOM	1002	CG2	ILE	A	130	17.317	37.091	19.030	1.00	46.63 C
ATOM	1003	CD1	ILE	A	130	17.934	38.126	16.313	1.00	58.84 C
ATOM	1004	N	ILE	A	131	14.681	38.675	19.568	1.00	45.61 N
ATOM	1005	CA	ILE	A	131	13.707	38.318	20.588	1.00	50.29 C
ATOM	1006	C	ILE	A	131	13.352	36.859	20.427	1.00	33.83 C
ATOM	1007	O	ILE	A	131	12.993	36.426	19.330	1.00	50.28 O
ATOM	1008	CB	ILE	A	131	12.374	39.104	20.474	1.00	55.23 C
ATOM	1009	CG1	ILE	A	131	12.620	40.610	20.479	1.00	61.34 C
ATOM	1010	CG2	ILE	A	131	11.470	38.737	21.647	1.00	58.84 C
ATOM	1011	CD1	ILE	A	131	12.630	41.236	19.085	1.00	60.34 C
ATOM	1012	N	TRP	A	132	13.437	36.108	21.520	1.00	38.49 N
ATOM	1013	CA	TRP	A	132	13.095	34.692	21.510	1.00	46.49 C
ATOM	1014	C	TRP	A	132	11.668	34.498	22.042	1.00	48.20 C
ATOM	1015	O	TRP	A	132	11.343	34.949	23.133	1.00	45.37 O
ATOM	1016	CB	TRP	A	132	14.085	33.898	22.372	1.00	39.62 C
ATOM	1017	CG	TRP	A	132	15.384	33.632	21.653	1.00	39.42 C

Figure 2 (Table 2 (page 26))

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ATOM   1018  CD1 TRP A 132      16.536  34.369  21.728  1.00 36.55 C
ATOM   1019  CD2 TRP A 132      15.645  32.570  20.726  1.00 29.03 C
ATOM   1020  NE1 TRP A 132      17.502  33.826  20.901  1.00 34.64 N
ATOM   1021  CE2 TRP A 132      16.985  32.725  20.278  1.00 35.20 C
ATOM   1022  CE3 TRP A 132      14.883  31.502  20.229  1.00 33.72 C
ATOM   1023  CZ2 TRP A 132      17.572  31.848  19.364  1.00 32.11 C
ATOM   1024  CZ3 TRP A 132      15.470  30.632  19.318  1.00 35.81 C
ATOM   1025  CH2 TRP A 132      16.809  30.814  18.893  1.00 33.40 C
ATOM   1026  N   LYS A 133      10.838  33.809  21.266  1.00 51.27 N
ATOM   1027  CA  LYS A 133       9.451  33.579  21.645  1.00 57.47 C
ATOM   1028  C   LYS A 133       9.043  32.124  21.741  1.00 59.45 C
ATOM   1029  O   LYS A 133       9.408  31.298  20.903  1.00 53.79 O
ATOM   1030  CB  LYS A 133       8.518  34.267  20.650  1.00 55.78 C
ATOM   1031  CG  LYS A 133       8.672  35.771  20.593  1.00 66.61 C
ATOM   1032  CD  LYS A 133       7.816  36.347  19.483  1.00 76.13 C
ATOM   1033  CE  LYS A 133       7.989  37.857  19.385  1.00 82.76 C
ATOM   1034  NZ  LYS A 133       7.076  38.469  18.372  1.00 81.20 N
ATOM   1035  N   HIS A 134       8.274  31.824  22.781  1.00 63.05 N
ATOM   1036  CA  HIS A 134       7.757  30.481  22.990  1.00 66.48 C
ATOM   1037  C   HIS A 134       6.265  30.612  23.220  1.00 77.89 C
ATOM   1038  O   HIS A 134       5.832  31.403  24.067  1.00 63.07 O
ATOM   1039  CB  HIS A 134       8.370  29.816  24.221  1.00 70.22 C
ATOM   1040  CG  HIS A 134       8.006  28.368  24.367  1.00 72.09 C
ATOM   1041  ND1 HIS A 134       8.057  27.704  25.574  1.00 72.16 N
ATOM   1042  CD2 HIS A 134       7.622  27.448  23.447  1.00 73.41 C
ATOM   1043  CE1 HIS A 134       7.723  26.440  25.392  1.00 77.82 C
ATOM   1044  NE2 HIS A 134       7.454  26.257  24.112  1.00 78.13 N
ATOM   1045  N   LYS A 135       5.488  29.843  22.461  1.00 81.08 N
ATOM   1046  CA  LYS A 135       4.034  29.850  22.574  1.00 91.79 C
ATOM   1047  C   LYS A 135       3.435  31.264  22.532  1.00 92.61 C
ATOM   1048  O   LYS A 135       2.397  31.511  23.139  1.00 95.56 O
ATOM   1049  CB  LYS A 135       3.608  29.135  23.870  1.00 90.50 C
ATOM   1050  CG  LYS A 135       3.832  29.955  25.143  1.00 96.62 C
ATOM   1051  CD  LYS A 135       3.541  29.173  26.414  1.00 94.31 C
ATOM   1052  CE  LYS A 135       3.714  30.058  27.643  1.00 94.84 C
ATOM   1053  NZ  LYS A 135       3.553  29.294  28.915  1.00 95.67 N
ATOM   1054  N   GLY A 136       4.082  32.194  21.828  1.00 91.50 N
ATOM   1055  CA  GLY A 136       3.553  33.551  21.741  1.00 88.54 C
ATOM   1056  C   GLY A 136       4.256  34.597  22.589  1.00 85.72 C
ATOM   1057  O   GLY A 136       4.366  35.754  22.187  1.00 89.77 O
ATOM   1058  N   ARG A 137       4.734  34.184  23.757  1.00 82.42 N
ATOM   1059  CA  ARG A 137       5.426  35.064  24.698  1.00 83.81 C
ATOM   1060  C   ARG A 137       6.867  35.398  24.329  1.00 80.74 C
ATOM   1061  O   ARG A 137       7.372  35.029  23.272  1.00 83.63 O
ATOM   1062  CB  ARG A 137       5.448  34.419  26.090  1.00 90.23 C
ATOM   1063  CG  ARG A 137       4.111  34.360  26.790  1.00 99.62 C
ATOM   1064  CD  ARG A 137       3.856  35.652  27.530  1.00105.25 C
ATOM   1065  NE  ARG A 137       2.445  36.009  27.526  1.00113.79 N
ATOM   1066  CZ  ARG A 137       1.973  37.181  27.937  1.00114.75 C
ATOM   1067  NH1 ARG A 137       2.805  38.109  28.390  1.00116.01 N
ATOM   1068  NH2 ARG A 137       0.672  37.432  27.883  1.00117.60 N
ATOM   1069  N   ASP A 138       7.510  36.116  25.241  1.00 76.46 N
ATOM   1070  CA  ASP A 138       8.907  36.497  25.132  1.00 75.03 C
ATOM   1071  C   ASP A 138       9.464  35.773  26.328  1.00 76.03 C
ATOM   1072  O   ASP A 138       9.139  36.102  27.476  1.00 73.85 O
ATOM   1073  CB  ASP A 138       9.107  38.000  25.318  1.00 77.22 C
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Figure 2 (Table 2 (page 27))

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ATOM   1074  CG  ASP A 138      10.578  38.403  25.275  1.00 77.41 C
ATOM   1075  OD1 ASP A 138      11.410  37.736  25.931  1.00 76.27 O
ATOM   1076  OD2 ASP A 138      10.906  39.394  24.590  1.00 67.17 O
ATOM   1077  N   VAL A 139      10.292  34.776  26.069  1.00 63.30 N
ATOM   1078  CA  VAL A 139      10.838  33.992  27.152  1.00 58.22 C
ATOM   1079  C   VAL A 139      11.541  34.814  28.224  1.00 60.55 C
ATOM   1080  O   VAL A 139      11.799  34.320  29.321  1.00 71.06 O
ATOM   1081  CB  VAL A 139      11.785  32.935  26.595  1.00 62.13 C
ATOM   1082  CG1 VAL A 139      11.091  32.195  25.469  1.00 55.43 C
ATOM   1083  CG2 VAL A 139      13.068  33.588  26.091  1.00 47.09 C
ATOM   1084  N   ILE A 140      11.841  36.070  27.918  1.00 66.18 N
ATOM   1085  CA  ILE A 140      12.519  36.924  28.878  1.00 73.19 C
ATOM   1086  C   ILE A 140      11.594  37.514  29.925  1.00 77.32 C
ATOM   1087  O   ILE A 140      11.822  37.370  31.123  1.00 79.51 O
ATOM   1088  CB  ILE A 140      13.229  38.098  28.183  1.00 75.30 C
ATOM   1089  CG1 ILE A 140      14.357  37.569  27.300  1.00 79.57 C
ATOM   1090  CG2 ILE A 140      13.789  39.062  29.227  1.00 84.41 C
ATOM   1091  CD1 ILE A 140      15.381  36.752  28.065  1.00 75.80 C
ATOM   1092  N   LEU A 141      10.553  38.194  29.468  1.00 85.78 N
ATOM   1093  CA  LEU A 141       9.632  38.838  30.384  1.00 97.07 C
ATOM   1094  C   LEU A 141       8.966  37.937  31.409  1.00101.56 C
ATOM   1095  O   LEU A 141       8.177  38.408  32.225  1.00107.39 O
ATOM   1096  CB  LEU A 141       8.571  39.615  29.608  1.00101.80 C
ATOM   1097  CG  LEU A 141       9.106  40.905  28.991  1.00106.45 C
ATOM   1098  CD1 LEU A 141       7.949  41.736  28.461  1.00108.62 C
ATOM   1099  CD2 LEU A 141       9.882  41.699  30.046  1.00104.45 C
ATOM   1100  N   LYS A 142       9.276  36.650  31.384  1.00101.47 N
ATOM   1101  CA  LYS A 142       8.689  35.751  32.362  1.00101.64 C
ATOM   1102  C   LYS A 142       9.660  35.560  33.527  1.00101.85 C
ATOM   1103  O   LYS A 142       9.262  35.339  34.675  1.00105.32 O
ATOM   1104  CB  LYS A 142       8.346  34.404  31.702  1.00100.75 C
ATOM   1105  CG  LYS A 142       9.525  33.643  31.098  1.00 98.61 C
ATOM   1106  CD  LYS A 142       8.997  32.520  30.208  1.00 93.54 C
ATOM   1107  CE  LYS A 142      10.082  31.550  29.747  1.00 96.37 C
ATOM   1108  NZ  LYS A 142       9.503  30.522  28.822  1.00 91.06 N
ATOM   1109  N   LYS A 143      10.940  35.703  33.223  1.00102.59 N
ATOM   1110  CA  LYS A 143      11.992  35.519  34.206  1.00104.90 C
ATOM   1111  C   LYS A 143      11.852  34.206  34.942  1.00100.79 C
ATOM   1112  O   LYS A 143      11.372  34.122  36.080  1.00100.29 O
ATOM   1113  CB  LYS A 143      12.059  36.672  35.207  1.00107.17 C
ATOM   1114  CG  LYS A 143      13.224  36.510  36.183  1.00113.10 C
ATOM   1115  CD  LYS A 143      14.559  36.248  35.522  1.00116.78 C
ATOM   1116  CE  LYS A 143      15.786  36.228  36.466  1.00123.03 C
ATOM   1117  NZ  LYS A 143      17.123  36.187  35.780  1.00119.60 N
ATOM   1118  N   ASP A 144      12.237  33.182  34.199  1.00 94.81 N
ATOM   1119  CA  ASP A 144      12.319  31.828  34.669  1.00 85.45 C
ATOM   1120  C   ASP A 144      13.827  31.840  34.531  1.00 79.96 C
ATOM   1121  O   ASP A 144      14.365  31.687  33.436  1.00 88.63 O
ATOM   1122  CB  ASP A 144      11.718  30.833  33.677  1.00 85.69 C
ATOM   1123  CG  ASP A 144      11.884  29.398  34.137  1.00 89.87 C
ATOM   1124  OD1 ASP A 144      12.989  29.060  34.609  1.00 90.66 O
ATOM   1125  OD2 ASP A 144      10.913  28.608  34.041  1.00101.36 O
ATOM   1126  N   VAL A 145      14.490  32.118  35.642  1.00 68.69 N
ATOM   1127  CA  VAL A 145      15.946  32.226  35.721  1.00 67.87 C
ATOM   1128  C   VAL A 145      16.758  31.316  34.795  1.00 55.99 C
ATOM   1129  O   VAL A 145      17.915  31.598  34.490  1.00 61.04 O
```

Figure 2 (Table 2 (page 28))

ATOM	1130	CB	VAL	A	145	16.415	31.974	37.167	1.00	76.83 C
ATOM	1131	CG1	VAL	A	145	15.901	33.082	38.076	1.00	76.29 C
ATOM	1132	CG2	VAL	A	145	15.902	30.617	37.655	1.00	77.74 C
ATOM	1133	N	ARG	A	146	16.148	30.227	34.349	1.00	52.68 N
ATOM	1134	CA	ARG	A	146	16.839	29.283	33.493	1.00	56.85 C
ATOM	1135	C	ARG	A	146	16.984	29.771	32.055	1.00	48.40 C
ATOM	1136	O	ARG	A	146	17.808	29.258	31.311	1.00	46.31 O
ATOM	1137	CB	ARG	A	146	16.121	27.925	33.538	1.00	44.42 C
ATOM	1138	CG	ARG	A	146	16.235	27.242	34.901	1.00	53.27 C
ATOM	1139	CD	ARG	A	146	15.613	25.846	34.911	1.00	47.00 C
ATOM	1140	NE	ARG	A	146	14.253	25.864	34.388	1.00	43.57 N
ATOM	1141	CZ	ARG	A	146	13.898	25.279	33.253	1.00	53.19 C
ATOM	1142	NH1	ARG	A	146	14.810	24.627	32.533	1.00	46.06 N
ATOM	1143	NH2	ARG	A	146	12.646	25.359	32.825	1.00	49.59 N
ATOM	1144	N	PHE	A	147	16.190	30.766	31.680	1.00	49.96 N
ATOM	1145	CA	PHE	A	147	16.233	31.297	30.330	1.00	55.08 C
ATOM	1146	C	PHE	A	147	17.068	32.568	30.213	1.00	55.40 C
ATOM	1147	O	PHE	A	147	16.837	33.551	30.916	1.00	58.84 O
ATOM	1148	CB	PHE	A	147	14.815	31.536	29.828	1.00	47.49 C
ATOM	1149	CG	PHE	A	147	14.003	30.271	29.679	1.00	55.00 C
ATOM	1150	CD1	PHE	A	147	13.520	29.598	30.796	1.00	50.35 C
ATOM	1151	CD2	PHE	A	147	13.730	29.747	28.416	1.00	49.95 C
ATOM	1152	CE1	PHE	A	147	12.773	28.416	30.654	1.00	61.13 C
ATOM	1153	CE2	PHE	A	147	12.986	28.571	28.265	1.00	53.83 C
ATOM	1154	CZ	PHE	A	147	12.508	27.905	29.386	1.00	56.75 C
ATOM	1155	N	ILE	A	148	18.038	32.536	29.307	1.00	50.18 N
ATOM	1156	CA	ILE	A	148	18.940	33.661	29.097	1.00	53.42 C
ATOM	1157	C	ILE	A	148	19.348	33.856	27.636	1.00	45.25 C
ATOM	1158	O	ILE	A	148	19.659	32.899	26.944	1.00	44.46 O
ATOM	1159	CB	ILE	A	148	20.233	33.463	29.908	1.00	55.88 C
ATOM	1160	CG1	ILE	A	148	19.907	33.427	31.399	1.00	65.94 C
ATOM	1161	CG2	ILE	A	148	21.231	34.573	29.597	1.00	61.53 C
ATOM	1162	CD1	ILE	A	148	21.093	33.081	32.279	1.00	69.07 C
ATOM	1163	N	VAL	A	149	19.337	35.099	27.172	1.00	37.73 N
ATOM	1164	CA	VAL	A	149	19.764	35.381	25.817	1.00	42.64 C
ATOM	1165	C	VAL	A	149	21.236	35.794	25.962	1.00	46.84 C
ATOM	1166	O	VAL	A	149	21.552	36.756	26.655	1.00	47.29 O
ATOM	1167	CB	VAL	A	149	18.929	36.512	25.185	1.00	42.61 C
ATOM	1168	CG1	VAL	A	149	19.472	36.844	23.791	1.00	44.21 C
ATOM	1169	CG2	VAL	A	149	17.444	36.067	25.064	1.00	43.57 C
ATOM	1170	N	LEU	A	150	22.127	35.036	25.328	1.00	40.34 N
ATOM	1171	CA	LEU	A	150	23.568	35.289	25.400	1.00	42.16 C
ATOM	1172	C	LEU	A	150	24.030	36.450	24.524	1.00	47.24 C
ATOM	1173	O	LEU	A	150	23.262	36.965	23.723	1.00	39.70 O
ATOM	1174	CB	LEU	A	150	24.305	34.019	25.001	1.00	36.82 C
ATOM	1175	CG	LEU	A	150	23.885	32.825	25.860	1.00	50.79 C
ATOM	1176	CD1	LEU	A	150	24.330	31.505	25.225	1.00	45.07 C
ATOM	1177	CD2	LEU	A	150	24.473	32.999	27.252	1.00	55.15 C
ATOM	1178	N	SER	A	151	25.295	36.849	24.666	1.00	50.63 N
ATOM	1179	CA	SER	A	151	25.849	37.953	23.880	1.00	44.74 C
ATOM	1180	C	SER	A	151	25.770	37.710	22.365	1.00	37.06 C
ATOM	1181	O	SER	A	151	25.651	38.663	21.587	1.00	49.84 O
ATOM	1182	CB	SER	A	151	27.320	38.200	24.273	1.00	45.09 C
ATOM	1183	OG	SER	A	151	28.150	37.144	23.792	1.00	45.86 O
ATOM	1184	N	ASN	A	152	25.866	36.455	21.937	1.00	38.65 N
ATOM	1185	CA	ASN	A	152	25.784	36.140	20.506	1.00	40.49 C

Figure 2 (Table 2 (page 29))

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ATOM   1186  C   ASN A 152      24.321  35.998  20.073  1.00 40.22 C
ATOM   1187  O   ASN A 152      24.036  35.583  18.936  1.00 34.75 O
ATOM   1188  CB  ASN A 152      26.476  34.821  20.207  1.00 39.82 C
ATOM   1189  CG  ASN A 152      26.097  33.752  21.199  1.00 54.90 C
ATOM   1190  OD1 ASN A 152      24.972  33.739  21.694  1.00 45.34 O
ATOM   1191  ND2 ASN A 152      27.029  32.850  21.504  1.00 46.13 N
ATOM   1192  N   ASN A 153      23.410  36.309  20.990  1.00 38.94 N
ATOM   1193  CA  ASN A 153      21.969  36.213  20.740  1.00 45.44 C
ATOM   1194  C   ASN A 153      21.352  34.827  20.723  1.00 42.99 C
ATOM   1195  O   ASN A 153      20.171  34.674  20.414  1.00 38.19 O
ATOM   1196  CB  ASN A 153      21.589  36.964  19.469  1.00 42.88 C
ATOM   1197  CG  ASN A 153      21.665  38.468  19.660  1.00 49.74 C
ATOM   1198  OD1 ASN A 153      21.300  38.990  20.720  1.00 57.35 O
ATOM   1199  ND2 ASN A 153      22.130  39.171  18.645  1.00 53.13 N
ATOM   1200  N   TYR A 154      22.121  33.810  21.080  1.00 31.78 N
ATOM   1201  CA  TYR A 154      21.563  32.463  21.151  1.00 37.05 C
ATOM   1202  C   TYR A 154      20.707  32.352  22.418  1.00 36.11 C
ATOM   1203  O   TYR A 154      20.918  33.107  23.357  1.00 35.56 O
ATOM   1204  CB  TYR A 154      22.675  31.425  21.247  1.00 35.50 C
ATOM   1205  CG  TYR A 154      23.535  31.329  20.021  1.00 40.10 C
ATOM   1206  CD1 TYR A 154      24.703  30.565  20.037  1.00 33.69 C
ATOM   1207  CD2 TYR A 154      23.179  31.990  18.837  1.00 35.06 C
ATOM   1208  CE1 TYR A 154      25.505  30.457  18.899  1.00 38.35 C
ATOM   1209  CE2 TYR A 154      23.979  31.892  17.676  1.00 34.58 C
ATOM   1210  CZ  TYR A 154      25.143  31.119  17.726  1.00 46.30 C
ATOM   1211  OH  TYR A 154      25.954  31.005  16.618  1.00 43.90 O
ATOM   1212  N   LEU A 155      19.757  31.415  22.450  1.00 37.10 N
ATOM   1213  CA  LEU A 155      18.936  31.237  23.650  1.00 33.06 C
ATOM   1214  C   LEU A 155      19.514  30.121  24.496  1.00 25.37 C
ATOM   1215  O   LEU A 155      19.688  28.989  24.037  1.00 33.57 O
ATOM   1216  CB  LEU A 155      17.482  30.866  23.303  1.00 33.13 C
ATOM   1217  CG  LEU A 155      16.635  30.561  24.545  1.00 39.86 C
ATOM   1218  CD1 LEU A 155      16.673  31.752  25.480  1.00 39.38 C
ATOM   1219  CD2 LEU A 155      15.185  30.269  24.142  1.00 35.14 C
ATOM   1220  N   GLN A 156      19.802  30.437  25.746  1.00 34.79 N
ATOM   1221  CA  GLN A 156      20.327  29.432  26.638  1.00 30.99 C
ATOM   1222  C   GLN A 156      19.212  28.964  27.568  1.00 33.82 C
ATOM   1223  O   GLN A 156      18.545  29.792  28.205  1.00 38.51 O
ATOM   1224  CB  GLN A 156      21.454  30.010  27.507  1.00 36.98 C
ATOM   1225  CG  GLN A 156      22.028  28.974  28.478  1.00 52.10 C
ATOM   1226  CD  GLN A 156      23.034  29.556  29.461  1.00 59.17 C
ATOM   1227  OE1 GLN A 156      22.750  30.542  30.134  1.00 58.98 O
ATOM   1228  NE2 GLN A 156      24.207  28.934  29.558  1.00 56.95 N
ATOM   1229  N   ILE A 157      19.012  27.651  27.655  1.00 35.15 N
ATOM   1230  CA  ILE A 157      18.001  27.104  28.570  1.00 39.14 C
ATOM   1231  C   ILE A 157      18.737  26.177  29.530  1.00 40.54 C
ATOM   1232  O   ILE A 157      19.028  25.030  29.189  1.00 41.38 O
ATOM   1233  CB  ILE A 157      16.928  26.304  27.832  1.00 36.32 C
ATOM   1234  CG1 ILE A 157      16.195  27.208  26.843  1.00 32.60 C
ATOM   1235  CG2 ILE A 157      15.943  25.728  28.842  1.00 42.84 C
ATOM   1236  CD1 ILE A 157      15.181  26.458  25.983  1.00 40.70 C
ATOM   1237  N   ARG A 158      19.068  26.674  30.718  1.00 38.99 N
ATOM   1238  CA  ARG A 158      19.804  25.857  31.673  1.00 45.51 C
ATOM   1239  C   ARG A 158      18.982  24.711  32.273  1.00 43.75 C
ATOM   1240  O   ARG A 158      17.781  24.851  32.484  1.00 47.32 O
ATOM   1241  CB  ARG A 158      20.381  26.749  32.778  1.00 53.96 C
```

Figure 2 (Table 2 (page 30))

ATOM	1242	CG	ARG	A	158	21.475	27.697	32.272	1.00	70.32	C
ATOM	1243	CD	ARG	A	158	22.155	28.453	33.405	1.00	65.23	C
ATOM	1244	NE	ARG	A	158	21.287	29.449	34.012	1.00	68.48	N
ATOM	1245	CZ	ARG	A	158	21.572	30.079	35.147	1.00	75.70	C
ATOM	1246	NH1	ARG	A	158	22.704	29.808	35.792	1.00	65.00	N
ATOM	1247	NH2	ARG	A	158	20.724	30.973	35.641	1.00	71.67	N
ATOM	1248	N	GLY	A	159	19.653	23.589	32.544	1.00	47.20	N
ATOM	1249	CA	GLY	A	159	18.998	22.415	33.096	1.00	48.68	C
ATOM	1250	C	GLY	A	159	17.731	22.133	32.317	1.00	50.27	C
ATOM	1251	O	GLY	A	159	16.658	21.983	32.897	1.00	44.17	O
ATOM	1252	N	ILE	A	160	17.847	22.050	30.997	1.00	46.11	N
ATOM	1253	CA	ILE	A	160	16.664	21.831	30.189	1.00	39.12	C
ATOM	1254	C	ILE	A	160	15.872	20.590	30.606	1.00	46.02	C
ATOM	1255	O	ILE	A	160	16.434	19.514	30.840	1.00	35.03	O
ATOM	1256	CB	ILE	A	160	17.013	21.755	28.702	1.00	34.52	C
ATOM	1257	CG1	ILE	A	160	15.727	21.917	27.874	1.00	37.12	C
ATOM	1258	CG2	ILE	A	160	17.679	20.446	28.376	1.00	34.14	C
ATOM	1259	CD1	ILE	A	160	15.993	22.199	26.392	1.00	28.22	C
ATOM	1260	N	LYS	A	161	14.557	20.767	30.692	1.00	42.18	N
ATOM	1261	CA	LYS	A	161	13.631	19.710	31.089	1.00	47.02	C
ATOM	1262	C	LYS	A	161	12.855	19.202	29.899	1.00	43.66	C
ATOM	1263	O	LYS	A	161	12.686	19.908	28.899	1.00	41.53	O
ATOM	1264	CB	LYS	A	161	12.599	20.236	32.095	1.00	49.68	C
ATOM	1265	CG	LYS	A	161	13.156	20.896	33.337	1.00	55.48	C
ATOM	1266	CD	LYS	A	161	12.002	21.450	34.178	1.00	65.12	C
ATOM	1267	CE	LYS	A	161	12.488	22.175	35.421	1.00	70.60	C
ATOM	1268	NZ	LYS	A	161	11.350	22.563	36.307	1.00	76.58	N
ATOM	1269	N	LYS	A	162	12.353	17.982	30.020	1.00	44.57	N
ATOM	1270	CA	LYS	A	162	11.560	17.383	28.956	1.00	47.82	C
ATOM	1271	C	LYS	A	162	10.372	18.311	28.670	1.00	43.43	C
ATOM	1272	O	LYS	A	162	9.914	18.427	27.535	1.00	44.67	O
ATOM	1273	CB	LYS	A	162	11.084	15.987	29.391	1.00	50.56	C
ATOM	1274	CG	LYS	A	162	10.298	15.208	28.339	1.00	50.30	C
ATOM	1275	CD	LYS	A	162	11.109	14.958	27.085	1.00	52.43	C
ATOM	1276	CE	LYS	A	162	10.279	14.227	26.051	1.00	60.58	C
ATOM	1277	NZ	LYS	A	162	10.963	14.149	24.731	1.00	59.55	N
ATOM	1278	N	THR	A	163	9.897	19.010	29.691	1.00	44.12	N
ATOM	1279	CA	THR	A	163	8.764	19.904	29.487	1.00	53.06	C
ATOM	1280	C	THR	A	163	9.140	21.234	28.833	1.00	55.60	C
ATOM	1281	O	THR	A	163	8.294	22.107	28.676	1.00	50.18	O
ATOM	1282	CB	THR	A	163	8.022	20.195	30.812	1.00	53.57	C
ATOM	1283	OG1	THR	A	163	8.942	20.712	31.780	1.00	55.40	O
ATOM	1284	CG2	THR	A	163	7.372	18.914	31.349	1.00	55.53	C
ATOM	1285	N	ASP	A	164	10.407	21.397	28.465	1.00	48.62	N
ATOM	1286	CA	ASP	A	164	10.826	22.628	27.810	1.00	42.03	C
ATOM	1287	C	ASP	A	164	10.764	22.477	26.299	1.00	44.90	C
ATOM	1288	O	ASP	A	164	10.821	23.470	25.573	1.00	48.57	O
ATOM	1289	CB	ASP	A	164	12.260	23.017	28.209	1.00	38.06	C
ATOM	1290	CG	ASP	A	164	12.358	23.525	29.631	1.00	36.69	C
ATOM	1291	OD1	ASP	A	164	11.469	24.295	30.052	1.00	49.63	O
ATOM	1292	OD2	ASP	A	164	13.337	23.168	30.327	1.00	44.71	O
ATOM	1293	N	GLU	A	165	10.639	21.251	25.798	1.00	44.64	N
ATOM	1294	CA	GLU	A	165	10.602	21.116	24.353	1.00	53.09	C
ATOM	1295	C	GLU	A	165	9.396	21.821	23.739	1.00	49.63	C
ATOM	1296	O	GLU	A	165	8.465	22.215	24.440	1.00	52.65	O
ATOM	1297	CB	GLU	A	165	10.681	19.650	23.909	1.00	50.75	C

Figure 2 (Table 2 (page 31))

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ATOM   1298  CG  GLU A 165       9.828  18.702  24.683  1.00 65.76 C
ATOM   1299  CD  GLU A 165       9.940  17.283  24.155  1.00 72.74 C
ATOM   1300  OE1 GLU A 165      11.040  16.884  23.691  1.00 69.18 O
ATOM   1301  OE2 GLU A 165       8.922  16.565  24.220  1.00 65.52 O
ATOM   1302  N   GLY A 166       9.451  22.002  22.424  1.00 48.94 N
ATOM   1303  CA  GLY A 166       8.405  22.700  21.701  1.00 55.73 C
ATOM   1304  C   GLY A 166       9.067  23.579  20.655  1.00 47.37 C
ATOM   1305  O   GLY A 166      10.256  23.419  20.340  1.00 47.39 O
ATOM   1306  N   THR A 167       8.317  24.517  20.112  0.50 34.99 N
ATOM   1307  CA  THR A 167       8.865  25.386  19.099  0.50 35.61 C
ATOM   1308  C   THR A 167       9.253  26.706  19.720  0.50 31.90 C
ATOM   1309  O   THR A 167       8.524  27.264  20.526  0.50 30.91 O
ATOM   1310  CB  THR A 167       7.849  25.623  18.006  0.50 40.53 C
ATOM   1311  OG1 THR A 167       6.633  26.081  18.602  0.50 51.84 O
ATOM   1312  CG2 THR A 167       7.574  24.332  17.258  0.50 26.00 C
ATOM   1313  N   TYR A 168      10.434  27.191  19.360  1.00 43.71 N
ATOM   1314  CA  TYR A 168      10.922  28.467  19.871  1.00 42.97 C
ATOM   1315  C   TYR A 168      11.183  29.372  18.689  1.00 38.98 C
ATOM   1316  O   TYR A 168      11.801  28.965  17.705  1.00 43.48 O
ATOM   1317  CB  TYR A 168      12.205  28.283  20.682  1.00 44.02 C
ATOM   1318  CG  TYR A 168      11.968  27.702  22.047  1.00 36.86 C
ATOM   1319  CD1 TYR A 168      11.676  26.353  22.206  1.00 38.88 C
ATOM   1320  CD2 TYR A 168      12.000  28.512  23.179  1.00 36.72 C
ATOM   1321  CE1 TYR A 168      11.419  25.821  23.466  1.00 41.93 C
ATOM   1322  CE2 TYR A 168      11.739  27.997  24.440  1.00 42.88 C
ATOM   1323  CZ  TYR A 168      11.451  26.652  24.576  1.00 43.41 C
ATOM   1324  OH  TYR A 168      11.193  26.139  25.824  1.00 40.88 O
ATOM   1325  N   ARG A 169      10.715  30.610  18.787  1.00 44.05 N
ATOM   1326  CA  ARG A 169      10.871  31.533  17.681  1.00 41.18 C
ATOM   1327  C   ARG A 169      12.013  32.526  17.868  1.00 36.73 C
ATOM   1328  O   ARG A 169      12.102  33.216  18.877  1.00 40.52 O
ATOM   1329  CB  ARG A 169       9.552  32.289  17.444  1.00 50.40 C
ATOM   1330  CG  ARG A 169       9.655  33.416  16.430  1.00 60.69 C
ATOM   1331  CD  ARG A 169       8.284  33.861  15.925  1.00 46.23 C
ATOM   1332  NE  ARG A 169       7.716  32.865  15.022  1.00 56.58 N
ATOM   1333  CZ  ARG A 169       6.535  32.984  14.420  1.00 71.77 C
ATOM   1334  NH1 ARG A 169       5.785  34.064  14.621  1.00 58.65 N
ATOM   1335  NH2 ARG A 169       6.101  32.015  13.618  1.00 59.89 N
ATOM   1336  N   CYS A 170      12.888  32.576  16.875  1.00 42.37 N
ATOM   1337  CA  CYS A 170      13.998  33.506  16.919  1.00 45.65 C
ATOM   1338  C   CYS A 170      13.546  34.667  16.025  1.00 31.99 C
ATOM   1339  O   CYS A 170      13.423  34.505  14.810  1.00 41.21 O
ATOM   1340  CB  CYS A 170      15.253  32.840  16.357  1.00 42.01 C
ATOM   1341  SG  CYS A 170      16.748  33.898  16.241  1.00 52.42 S
ATOM   1342  N   GLU A 171      13.289  35.820  16.635  1.00 44.29 N
ATOM   1343  CA  GLU A 171      12.830  36.978  15.879  1.00 49.65 C
ATOM   1344  C   GLU A 171      13.814  38.129  15.844  1.00 40.68 C
ATOM   1345  O   GLU A 171      14.218  38.663  16.885  1.00 45.31 O
ATOM   1346  CB  GLU A 171      11.503  37.502  16.426  1.00 47.28 C
ATOM   1347  CG  GLU A 171      10.905  38.616  15.560  1.00 57.47 C
ATOM   1348  CD  GLU A 171       9.580  39.147  16.096  1.00 65.00 C
ATOM   1349  OE1 GLU A 171       9.593  39.989  17.028  1.00 62.15 O
ATOM   1350  OE2 GLU A 171       8.531  38.707  15.584  1.00 54.66 O
ATOM   1351  N   GLY A 172      14.163  38.525  14.625  1.00 46.09 N
ATOM   1352  CA  GLY A 172      15.086  39.624  14.436  1.00 49.63 C
ATOM   1353  C   GLY A 172      14.388  40.872  13.930  1.00 46.92 C
```

Figure 2 (Table 2 (page 32))

ATOM	1354	O	GLY	A	172	13.557	40.812	13.014	1.00	50.71 O
ATOM	1355	N	ARG	A	173	14.753	41.998	14.535	1.00	40.06 N
ATOM	1356	CA	ARG	A	173	14.222	43.309	14.215	1.00	44.00 C
ATOM	1357	C	ARG	A	173	15.335	44.350	14.038	1.00	56.42 C
ATOM	1358	O	ARG	A	173	16.328	44.354	14.768	1.00	47.64 O
ATOM	1359	CB	ARG	A	173	13.310	43.800	15.345	1.00	42.90 C
ATOM	1360	CG	ARG	A	173	12.048	42.970	15.527	1.00	41.21 C
ATOM	1361	CD	ARG	A	173	11.096	43.649	16.488	1.00	49.33 C
ATOM	1362	NE	ARG	A	173	9.880	42.862	16.656	1.00	55.21 N
ATOM	1363	CZ	ARG	A	173	8.669	43.387	16.790	1.00	54.70 C
ATOM	1364	NH1	ARG	A	173	8.518	44.704	16.773	1.00	54.11 N
ATOM	1365	NH2	ARG	A	173	7.610	42.596	16.935	1.00	54.36 N
ATOM	1366	N	ILE	A	174	15.135	45.245	13.080	1.00	51.94 N
ATOM	1367	CA	ILE	A	174	16.068	46.331	12.821	1.00	48.52 C
ATOM	1368	C	ILE	A	174	15.228	47.591	12.902	1.00	42.65 C
ATOM	1369	O	ILE	A	174	14.485	47.901	11.973	1.00	40.81 O
ATOM	1370	CB	ILE	A	174	16.687	46.193	11.436	1.00	51.33 C
ATOM	1371	CG1	ILE	A	174	17.536	44.921	11.395	1.00	62.03 C
ATOM	1372	CG2	ILE	A	174	17.536	47.417	11.128	1.00	57.79 C
ATOM	1373	CD1	ILE	A	174	18.075	44.586	10.042	1.00	60.04 C
ATOM	1374	N	LEU	A	175	15.348	48.327	14.004	1.00	43.83 N
ATOM	1375	CA	LEU	A	175	14.514	49.513	14.203	1.00	50.67 C
ATOM	1376	C	LEU	A	175	14.502	50.558	13.102	1.00	53.85 C
ATOM	1377	O	LEU	A	175	13.435	51.017	12.694	1.00	54.58 O
ATOM	1378	CB	LEU	A	175	14.853	50.223	15.520	1.00	52.93 C
ATOM	1379	CG	LEU	A	175	14.067	51.544	15.693	1.00	69.90 C
ATOM	1380	CD1	LEU	A	175	12.539	51.287	15.592	1.00	58.23 C
ATOM	1381	CD2	LEU	A	175	14.423	52.195	17.026	1.00	61.03 C
ATOM	1382	N	ALA	A	176	15.681	50.962	12.641	1.00	49.99 N
ATOM	1383	CA	ALA	A	176	15.753	51.981	11.605	1.00	51.23 C
ATOM	1384	C	ALA	A	176	14.902	51.629	10.385	1.00	45.44 C
ATOM	1385	O	ALA	A	176	14.347	52.518	9.739	1.00	57.30 O
ATOM	1386	CB	ALA	A	176	17.211	52.214	11.193	1.00	54.86 C
ATOM	1387	N	ARG	A	177	14.776	50.341	10.074	1.00	50.42 N
ATOM	1388	CA	ARG	A	177	13.987	49.924	8.917	1.00	45.08 C
ATOM	1389	C	ARG	A	177	12.641	49.302	9.269	1.00	48.67 C
ATOM	1390	O	ARG	A	177	11.862	48.974	8.377	1.00	45.39 O
ATOM	1391	CB	ARG	A	177	14.778	48.918	8.081	1.00	57.24 C
ATOM	1392	CG	ARG	A	177	16.084	49.467	7.544	1.00	64.35 C
ATOM	1393	CD	ARG	A	177	16.813	48.460	6.666	1.00	64.31 C
ATOM	1394	NE	ARG	A	177	17.880	49.138	5.939	1.00	77.29 N
ATOM	1395	CZ	ARG	A	177	17.889	49.331	4.625	1.00	58.44 C
ATOM	1396	NH1	ARG	A	177	16.892	48.883	3.873	1.00	54.23 N
ATOM	1397	NH2	ARG	A	177	18.884	50.009	4.074	1.00	72.33 N
ATOM	1398	N	GLY	A	178	12.373	49.130	10.562	1.00	44.96 N
ATOM	1399	CA	GLY	A	178	11.122	48.508	10.972	1.00	44.41 C
ATOM	1400	C	GLY	A	178	11.050	47.122	10.354	1.00	44.68 C
ATOM	1401	O	GLY	A	178	9.976	46.574	10.092	1.00	40.98 O
ATOM	1402	N	GLU	A	179	12.227	46.544	10.146	1.00	41.13 N
ATOM	1403	CA	GLU	A	179	12.363	45.240	9.513	1.00	46.62 C
ATOM	1404	C	GLU	A	179	12.204	44.076	10.496	1.00	46.51 C
ATOM	1405	O	GLU	A	179	12.710	44.116	11.619	1.00	46.07 O
ATOM	1406	CB	GLU	A	179	13.736	45.192	8.817	1.00	47.47 C
ATOM	1407	CG	GLU	A	179	14.011	44.049	7.852	1.00	52.61 C
ATOM	1408	CD	GLU	A	179	15.396	44.199	7.186	1.00	67.97 C
ATOM	1409	OE1	GLU	A	179	16.232	44.974	7.709	1.00	52.50 O

Figure 2 (Table 2 (page 33))

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ATOM   1410  OE2 GLU A 179      15.657  43.540   6.156  1.00 61.67 O
ATOM   1411  N   ILE A 180      11.504  43.037  10.044  1.00 46.98 N
ATOM   1412  CA  ILE A 180      11.260  41.843  10.844  1.00 44.57 C
ATOM   1413  C   ILE A 180      11.442  40.596  10.028  1.00 49.88 C
ATOM   1414  O   ILE A 180      11.018  40.531   8.878  1.00 50.41 O
ATOM   1415  CB  ILE A 180       9.820  41.784  11.371  1.00 60.91 C
ATOM   1416  CG1 ILE A 180       9.586  42.889  12.387  1.00 56.28 C
ATOM   1417  CG2 ILE A 180       9.544  40.416  11.996  1.00 58.36 C
ATOM   1418  CD1 ILE A 180       8.206  42.834  12.973  1.00 63.77 C
ATOM   1419  N   ASN A 181      12.088  39.607  10.632  1.00 49.49 N
ATOM   1420  CA  ASN A 181      12.269  38.308  10.010  1.00 44.31 C
ATOM   1421  C   ASN A 181      12.329  37.382  11.223  1.00 53.84 C
ATOM   1422  O   ASN A 181      12.789  37.776  12.297  1.00 49.42 O
ATOM   1423  CB  ASN A 181      13.555  38.240   9.189  1.00 50.86 C
ATOM   1424  CG  ASN A 181      13.527  37.117   8.165  1.00 58.63 C
ATOM   1425  OD1 ASN A 181      12.581  36.332   8.126  1.00 68.55 O
ATOM   1426  ND2 ASN A 181      14.567  37.031   7.331  1.00 62.99 N
ATOM   1427  N   PHE A 182      11.818  36.172  11.082  1.00 51.66 N
ATOM   1428  CA  PHE A 182      11.839  35.261  12.210  1.00 54.82 C
ATOM   1429  C   PHE A 182      12.052  33.843  11.711  1.00 62.75 C
ATOM   1430  O   PHE A 182      11.914  33.563  10.512  1.00 55.35 O
ATOM   1431  CB  PHE A 182      10.521  35.354  12.989  1.00 62.28 C
ATOM   1432  CG  PHE A 182       9.352  34.717  12.283  1.00 74.94 C
ATOM   1433  CD1 PHE A 182       9.292  33.333  12.120  1.00 82.11 C
ATOM   1434  CD2 PHE A 182       8.333  35.496  11.745  1.00 81.28 C
ATOM   1435  CE1 PHE A 182       8.244  32.733  11.429  1.00 84.02 C
ATOM   1436  CE2 PHE A 182       7.276  34.901  11.049  1.00 84.09 C
ATOM   1437  CZ  PHE A 182       7.236  33.516  10.892  1.00 83.03 C
ATOM   1438  N   LYS A 183      12.388  32.946  12.633  1.00 58.39 N
ATOM   1439  CA  LYS A 183      12.591  31.541  12.295  1.00 50.63 C
ATOM   1440  C   LYS A 183      12.106  30.678  13.459  1.00 53.23 C
ATOM   1441  O   LYS A 183      12.431  30.947  14.622  1.00 45.57 O
ATOM   1442  CB  LYS A 183      14.073  31.263  12.022  1.00 65.15 C
ATOM   1443  CG  LYS A 183      14.446  29.780  11.957  1.00 64.65 C
ATOM   1444  CD  LYS A 183      14.295  29.166  10.566  1.00 63.11 C
ATOM   1445  CE  LYS A 183      14.627  27.670  10.590  1.00 53.42 C
ATOM   1446  NZ  LYS A 183      15.665  27.264   9.599  1.00 53.61 N
ATOM   1447  N   ASP A 184      11.319  29.655  13.142  1.00 48.66 N
ATOM   1448  CA  ASP A 184      10.797  28.751  14.156  1.00 52.92 C
ATOM   1449  C   ASP A 184      11.722  27.567  14.333  1.00 45.71 C
ATOM   1450  O   ASP A 184      12.104  26.894  13.371  1.00 44.54 O
ATOM   1451  CB  ASP A 184       9.404  28.255  13.784  1.00 62.54 C
ATOM   1452  CG  ASP A 184       8.338  29.306  14.007  1.00 62.50 C
ATOM   1453  OD1 ASP A 184       8.407  30.010  15.038  1.00 56.56 O
ATOM   1454  OD2 ASP A 184       7.429  29.417  13.155  1.00 70.30 O
ATOM   1455  N   ILE A 185      12.085  27.313  15.576  1.00 40.93 N
ATOM   1456  CA  ILE A 185      12.993  26.219  15.849  1.00 39.71 C
ATOM   1457  C   ILE A 185      12.372  25.231  16.806  1.00 38.52 C
ATOM   1458  O   ILE A 185      11.958  25.590  17.909  1.00 38.65 O
ATOM   1459  CB  ILE A 185      14.326  26.752  16.417  1.00 41.45 C
ATOM   1460  CG1 ILE A 185      15.051  27.548  15.316  1.00 46.89 C
ATOM   1461  CG2 ILE A 185      15.199  25.580  16.922  1.00 37.86 C
ATOM   1462  CD1 ILE A 185      16.246  28.337  15.805  1.00 48.29 C
ATOM   1463  N   GLN A 186      12.291  23.984  16.355  1.00 42.25 N
ATOM   1464  CA  GLN A 186      11.744  22.916  17.181  1.00 41.47 C
ATOM   1465  C   GLN A 186      12.857  22.416  18.097  1.00 38.63 C
```

Figure 2 (Table 2 (page 34))

ATOM	1466	O	GLN	A	186	13.916	21.991	17.630	1.00	42.48	O
ATOM	1467	CB	GLN	A	186	11.247	21.755	16.307	1.00	52.01	C
ATOM	1468	CG	GLN	A	186	10.732	20.542	17.100	1.00	64.38	C
ATOM	1469	CD	GLN	A	186	10.353	19.348	16.204	1.00	79.51	C
ATOM	1470	OE1	GLN	A	186	10.873	19.202	15.092	1.00	79.17	O
ATOM	1471	NE2	GLN	A	186	9.465	18.481	16.701	1.00	80.31	N
ATOM	1472	N	VAL	A	187	12.610	22.457	19.398	1.00	43.44	N
ATOM	1473	CA	VAL	A	187	13.586	21.987	20.367	1.00	47.67	C
ATOM	1474	C	VAL	A	187	13.146	20.607	20.866	1.00	49.13	C
ATOM	1475	O	VAL	A	187	12.015	20.446	21.311	1.00	40.93	O
ATOM	1476	CB	VAL	A	187	13.675	22.939	21.583	1.00	42.03	C
ATOM	1477	CG1	VAL	A	187	14.563	22.315	22.652	1.00	41.16	C
ATOM	1478	CG2	VAL	A	187	14.224	24.300	21.154	1.00	38.03	C
ATOM	1479	N	ILE	A	188	14.035	19.621	20.785	1.00	41.32	N
ATOM	1480	CA	ILE	A	188	13.733	18.273	21.255	1.00	42.62	C
ATOM	1481	C	ILE	A	188	14.635	17.913	22.441	1.00	40.36	C
ATOM	1482	O	ILE	A	188	15.835	18.224	22.442	1.00	42.29	O
ATOM	1483	CB	ILE	A	188	13.945	17.213	20.142	1.00	45.03	C
ATOM	1484	CG1	ILE	A	188	13.002	17.475	18.967	1.00	41.79	C
ATOM	1485	CG2	ILE	A	188	13.687	15.806	20.702	1.00	46.59	C
ATOM	1486	CD1	ILE	A	188	13.267	16.566	17.763	1.00	40.92	C
ATOM	1487	N	VAL	A	189	14.050	17.285	23.455	1.00	36.36	N
ATOM	1488	CA	VAL	A	189	14.808	16.867	24.627	1.00	42.50	C
ATOM	1489	C	VAL	A	189	14.802	15.338	24.667	1.00	48.22	C
ATOM	1490	O	VAL	A	189	13.748	14.705	24.672	1.00	41.17	O
ATOM	1491	CB	VAL	A	189	14.206	17.455	25.921	1.00	44.30	C
ATOM	1492	CG1	VAL	A	189	14.945	16.930	27.125	1.00	39.49	C
ATOM	1493	CG2	VAL	A	189	14.304	18.966	25.894	1.00	40.56	C
ATOM	1494	N	ASN	A	190	15.993	14.754	24.665	1.00	40.63	N
ATOM	1495	CA	ASN	A	190	16.143	13.316	24.698	1.00	40.98	C
ATOM	1496	C	ASN	A	190	16.395	12.885	26.148	1.00	45.73	C
ATOM	1497	O	ASN	A	190	17.018	13.613	26.918	1.00	45.44	O
ATOM	1498	CB	ASN	A	190	17.285	12.908	23.752	1.00	40.78	C
ATOM	1499	CG	ASN	A	190	16.999	13.293	22.310	1.00	48.31	C
ATOM	1500	OD1	ASN	A	190	15.917	13.005	21.782	1.00	44.75	O
ATOM	1501	ND2	ASN	A	190	17.962	13.951	21.664	1.00	41.66	N
ATOM	1502	N	VAL	A	191	15.877	11.710	26.509	1.00	42.84	N
ATOM	1503	CA	VAL	A	191	15.982	11.151	27.863	1.00	39.39	C
ATOM	1504	C	VAL	A	191	16.683	9.802	27.788	1.00	39.64	C
ATOM	1505	O	VAL	A	191	16.261	8.910	27.043	1.00	47.40	O
ATOM	1506	CB	VAL	A	191	14.574	10.954	28.470	1.00	44.63	C
ATOM	1507	CG1	VAL	A	191	14.671	10.368	29.890	1.00	41.78	C
ATOM	1508	CG2	VAL	A	191	13.848	12.310	28.499	1.00	41.72	C
ATOM	1509	N	PRO	A	192	17.775	9.641	28.542	1.00	43.27	N
ATOM	1510	CA	PRO	A	192	18.578	8.416	28.596	1.00	45.21	C
ATOM	1511	C	PRO	A	192	17.722	7.224	28.990	1.00	42.00	C
ATOM	1512	O	PRO	A	192	16.783	7.355	29.763	1.00	42.35	O
ATOM	1513	CB	PRO	A	192	19.620	8.737	29.668	1.00	49.92	C
ATOM	1514	CG	PRO	A	192	19.690	10.204	29.687	1.00	49.81	C
ATOM	1515	CD	PRO	A	192	18.246	10.602	29.556	1.00	43.30	C
ATOM	1516	N	PRO	A	193	18.075	6.034	28.515	1.00	40.57	N
ATOM	1517	CA	PRO	A	193	17.301	4.848	28.838	1.00	39.79	C
ATOM	1518	C	PRO	A	193	17.516	4.372	30.256	1.00	43.45	C
ATOM	1519	O	PRO	A	193	18.552	4.666	30.864	1.00	44.20	O
ATOM	1520	CB	PRO	A	193	17.842	3.809	27.853	1.00	41.07	C
ATOM	1521	CG	PRO	A	193	18.661	4.630	26.843	1.00	46.01	C

Figure 2 (Table 2 (page 35))

ATOM	1522	CD	PRO	A	193	19.250	5.657	27.729	1.00	47.13	C
ATOM	1523	N	THR	A	194	16.516	3.665	30.779	1.00	45.04	N
ATOM	1524	CA	THR	A	194	16.614	2.987	32.075	1.00	48.33	C
ATOM	1525	C	THR	A	194	16.019	1.623	31.713	1.00	51.40	C
ATOM	1526	O	THR	A	194	15.124	1.529	30.848	1.00	41.84	O
ATOM	1527	CB	THR	A	194	15.792	3.630	33.225	1.00	48.61	C
ATOM	1528	OG1	THR	A	194	14.414	3.724	32.862	1.00	54.30	O
ATOM	1529	CG2	THR	A	194	16.338	4.992	33.574	1.00	57.24	C
ATOM	1530	N	VAL	A	195	16.507	0.565	32.352	1.00	48.50	N
ATOM	1531	CA	VAL	A	195	16.026	-0.760	32.017	1.00	45.60	C
ATOM	1532	C	VAL	A	195	16.083	-1.715	33.200	1.00	42.61	C
ATOM	1533	O	VAL	A	195	16.976	-1.644	34.021	1.00	46.25	O
ATOM	1534	CB	VAL	A	195	16.853	-1.346	30.840	1.00	42.93	C
ATOM	1535	CG1	VAL	A	195	18.314	-1.582	31.282	1.00	43.08	C
ATOM	1536	CG2	VAL	A	195	16.218	-2.635	30.339	1.00	43.46	C
ATOM	1537	N	GLN	A	196	15.104	-2.603	33.282	1.00	41.51	N
ATOM	1538	CA	GLN	A	196	15.070	-3.577	34.355	1.00	48.63	C
ATOM	1539	C	GLN	A	196	14.615	-4.928	33.817	1.00	46.66	C
ATOM	1540	O	GLN	A	196	13.706	-5.009	32.992	1.00	45.71	O
ATOM	1541	CB	GLN	A	196	14.119	-3.118	35.477	1.00	49.59	C
ATOM	1542	CG	GLN	A	196	14.693	-2.064	36.393	1.00	55.69	C
ATOM	1543	CD	GLN	A	196	13.790	-1.757	37.588	1.00	74.35	C
ATOM	1544	OE1	GLN	A	196	14.268	-1.328	38.639	1.00	74.51	O
ATOM	1545	NE2	GLN	A	196	12.482	-1.970	37.429	1.00	79.78	N
ATOM	1546	N	ALA	A	197	15.257	-5.991	34.282	1.00	40.70	N
ATOM	1547	CA	ALA	A	197	14.876	-7.329	33.873	1.00	39.75	C
ATOM	1548	C	ALA	A	197	13.550	-7.650	34.550	1.00	42.61	C
ATOM	1549	O	ALA	A	197	13.316	-7.246	35.687	1.00	48.54	O
ATOM	1550	CB	ALA	A	197	15.940	-8.333	34.313	1.00	39.72	C
ATOM	1551	N	ARG	A	198	12.671	-8.368	33.865	1.00	43.54	N
ATOM	1552	CA	ARG	A	198	11.403	-8.720	34.485	1.00	44.25	C
ATOM	1553	C	ARG	A	198	11.664	-9.866	35.479	1.00	53.02	C
ATOM	1554	O	ARG	A	198	11.018	-9.960	36.528	1.00	45.60	O
ATOM	1555	CB	ARG	A	198	10.392	-9.131	33.416	1.00	49.38	C
ATOM	1556	CG	ARG	A	198	8.967	-8.992	33.873	1.00	56.08	C
ATOM	1557	CD	ARG	A	198	7.991	-9.099	32.724	1.00	58.30	C
ATOM	1558	NE	ARG	A	198	7.873	-7.869	31.947	1.00	47.20	N
ATOM	1559	CZ	ARG	A	198	6.931	-7.675	31.030	1.00	54.23	C
ATOM	1560	NH1	ARG	A	198	6.038	-8.633	30.793	1.00	47.47	N
ATOM	1561	NH2	ARG	A	198	6.882	-6.541	30.339	1.00	50.85	N
ATOM	1562	N	GLN	A	199	12.625	-10.722	35.133	1.00	51.86	N
ATOM	1563	CA	GLN	A	199	13.047	-11.844	35.965	1.00	52.79	C
ATOM	1564	C	GLN	A	199	14.564	-11.926	35.871	1.00	50.17	C
ATOM	1565	O	GLN	A	199	15.107	-12.162	34.798	1.00	54.53	O
ATOM	1566	CB	GLN	A	199	12.447	-13.159	35.472	1.00	58.34	C
ATOM	1567	CG	GLN	A	199	10.941	-13.292	35.635	1.00	68.50	C
ATOM	1568	CD	GLN	A	199	10.498	-13.315	37.100	1.00	83.24	C
ATOM	1569	OE1	GLN	A	199	11.300	-13.596	37.996	1.00	85.74	O
ATOM	1570	NE2	GLN	A	199	9.214	-13.035	37.347	1.00	71.40	N
ATOM	1571	N	SER	A	200	15.247	-11.719	36.991	1.00	46.12	N
ATOM	1572	CA	SER	A	200	16.715	-11.753	37.042	1.00	50.15	C
ATOM	1573	C	SER	A	200	17.328	-13.157	37.004	1.00	47.60	C
ATOM	1574	O	SER	A	200	18.458	-13.350	36.541	1.00	49.49	O
ATOM	1575	CB	SER	A	200	17.194	-11.061	38.318	1.00	49.46	C
ATOM	1576	OG	SER	A	200	16.702	-9.737	38.384	1.00	76.11	O
ATOM	1577	N	ILE	A	201	16.576	-14.122	37.518	1.00	48.87	N

Figure 2 (Table 2 (page 36))

```
ATOM   1578  CA  ILE A 201      17.019 -15.504  37.591  1.00 50.62 C
ATOM   1579  C   ILE A 201      15.994 -16.400  36.925  1.00 47.35 C
ATOM   1580  O   ILE A 201      14.797 -16.328  37.216  1.00 51.41 O
ATOM   1581  CB  ILE A 201      17.181 -15.962  39.067  1.00 64.29 C
ATOM   1582  CG1 ILE A 201      18.080 -14.983  39.838  1.00 57.76 C
ATOM   1583  CG2 ILE A 201      17.768 -17.373  39.116  1.00 58.42 C
ATOM   1584  CD1 ILE A 201      19.476 -14.860  39.290  1.00 68.87 C
ATOM   1585  N   VAL A 202      16.469 -17.249  36.032  1.00 46.21 N
ATOM   1586  CA  VAL A 202      15.587 -18.157  35.339  1.00 49.25 C
ATOM   1587  C   VAL A 202      16.207 -19.540  35.336  1.00 47.17 C
ATOM   1588  O   VAL A 202      17.391 -19.687  35.045  1.00 43.79 O
ATOM   1589  CB  VAL A 202      15.371 -17.701  33.882  1.00 53.12 C
ATOM   1590  CG1 VAL A 202      14.436 -18.661  33.177  1.00 45.19 C
ATOM   1591  CG2 VAL A 202      14.820 -16.276  33.861  1.00 50.64 C
ATOM   1592  N   ASN A 203      15.393 -20.544  35.653  1.00 49.57 N
ATOM   1593  CA  ASN A 203      15.827 -21.937  35.680  1.00 51.28 C
ATOM   1594  C   ASN A 203      15.078 -22.676  34.575  1.00 55.81 C
ATOM   1595  O   ASN A 203      13.857 -22.541  34.440  1.00 50.57 O
ATOM   1596  CB  ASN A 203      15.473 -22.635  37.010  1.00 49.03 C
ATOM   1597  CG  ASN A 203      16.218 -22.067  38.217  1.00 47.83 C
ATOM   1598  OD1 ASN A 203      17.319 -21.530  38.105  1.00 47.54 O
ATOM   1599  ND2 ASN A 203      15.617 -22.217  39.390  1.00 44.22 N
ATOM   1600  N   ALA A 204      15.811 -23.487  33.825  1.00 53.79 N
ATOM   1601  CA  ALA A 204      15.249 -24.272  32.738  1.00 58.78 C
ATOM   1602  C   ALA A 204      15.827 -25.683  32.730  1.00 59.86 C
ATOM   1603  O   ALA A 204      16.909 -25.933  33.268  1.00 58.63 O
ATOM   1604  CB  ALA A 204      15.541 -23.592  31.408  1.00 54.08 C
ATOM   1605  N   THR A 205      15.088 -26.592  32.100  1.00 63.01 N
ATOM   1606  CA  THR A 205      15.483 -27.989  31.966  1.00 62.26 C
ATOM   1607  C   THR A 205      15.949 -28.248  30.546  1.00 59.60 C
ATOM   1608  O   THR A 205      15.282 -27.874  29.579  1.00 57.70 O
ATOM   1609  CB  THR A 205      14.323 -28.946  32.265  1.00 63.31 C
ATOM   1610  OG1 THR A 205      13.916 -28.799  33.634  1.00 64.86 O
ATOM   1611  CG2 THR A 205      14.760 -30.383  32.012  1.00 70.94 C
ATOM   1612  N   ALA A 206      17.089 -28.913  30.430  1.00 56.34 N
ATOM   1613  CA  ALA A 206      17.670 -29.203  29.134  1.00 60.33 C
ATOM   1614  C   ALA A 206      17.035 -30.352  28.375  1.00 64.54 C
ATOM   1615  O   ALA A 206      16.377 -31.228  28.940  1.00 68.98 O
ATOM   1616  CB  ALA A 206      19.156 -29.464  29.290  1.00 58.07 C
ATOM   1617  N   ASN A 207      17.246 -30.306  27.067  1.00 71.10 N
ATOM   1618  CA  ASN A 207      16.791 -31.322  26.140  1.00 71.82 C
ATOM   1619  C   ASN A 207      15.352 -31.788  26.216  1.00 70.92 C
ATOM   1620  O   ASN A 207      15.077 -32.971  26.023  1.00 73.91 O
ATOM   1621  CB  ASN A 207      17.724 -32.518  26.249  1.00 69.97 C
ATOM   1622  CG  ASN A 207      19.170 -32.119  26.105  1.00 75.29 C
ATOM   1623  OD1 ASN A 207      19.562 -31.531  25.097  1.00 81.94 O
ATOM   1624  ND2 ASN A 207      19.972 -32.421  27.115  1.00 80.72 N
ATOM   1625  N   LEU A 208      14.432 -30.877  26.496  1.00 67.07 N
ATOM   1626  CA  LEU A 208      13.026 -31.246  26.528  1.00 68.52 C
ATOM   1627  C   LEU A 208      12.347 -30.484  25.391  1.00 67.74 C
ATOM   1628  O   LEU A 208      11.122 -30.415  25.306  1.00 73.14 O
ATOM   1629  CB  LEU A 208      12.393 -30.904  27.877  1.00 68.09 C
ATOM   1630  CG  LEU A 208      12.930 -31.679  29.091  1.00 79.90 C
ATOM   1631  CD1 LEU A 208      12.105 -31.321  30.319  1.00 73.01 C
ATOM   1632  CD2 LEU A 208      12.854 -33.180  28.843  1.00 77.54 C
ATOM   1633  N   GLY A 209      13.175 -29.907  24.519  1.00 74.00 N
```

Figure 2 (Table 2 (page 37))

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ATOM   1634  CA  GLY A 209      12.694 -29.159  23.364  1.00 81.72 C
ATOM   1635  C   GLY A 209      11.907 -27.893  23.667  1.00 87.49 C
ATOM   1636  O   GLY A 209      11.241 -27.341  22.788  1.00 95.12 O
ATOM   1637  N   GLN A 210      11.992 -27.420  24.905  1.00 84.00 N
ATOM   1638  CA  GLN A 210      11.254 -26.230  25.299  1.00 82.13 C
ATOM   1639  C   GLN A 210      12.033 -24.922  25.205  1.00 74.00 C
ATOM   1640  O   GLN A 210      13.265 -24.922  25.132  1.00 71.75 O
ATOM   1641  CB  GLN A 210      10.703 -26.400  26.711  1.00 86.64 C
ATOM   1642  CG  GLN A 210      11.770 -26.685  27.754  1.00 92.84 C
ATOM   1643  CD  GLN A 210      11.215 -27.469  28.932  1.00 98.28 C
ATOM   1644  OE1 GLN A 210      10.047 -27.856  28.930  1.00102.57 O
ATOM   1645  NE2 GLN A 210      12.049 -27.714  29.938  1.00100.49 N
ATOM   1646  N   SER A 211      11.295 -23.810  25.212  1.00 73.42 N
ATOM   1647  CA  SER A 211      11.873 -22.470  25.101  1.00 68.89 C
ATOM   1648  C   SER A 211      11.749 -21.688  26.394  1.00 59.63 C
ATOM   1649  O   SER A 211      10.995 -22.044  27.297  1.00 58.00 O
ATOM   1650  CB  SER A 211      11.181 -21.680  23.978  1.00 69.06 C
ATOM   1651  OG  SER A 211      11.312 -22.319  22.719  1.00 75.29 O
ATOM   1652  N   VAL A 212      12.515 -20.616  26.479  1.00 62.83 N
ATOM   1653  CA  VAL A 212      12.470 -19.749  27.638  1.00 57.69 C
ATOM   1654  C   VAL A 212      12.482 -18.343  27.056  1.00 51.71 C
ATOM   1655  O   VAL A 212      13.140 -18.086  26.044  1.00 48.36 O
ATOM   1656  CB  VAL A 212      13.697 -19.965  28.554  1.00 58.76 C
ATOM   1657  CG1 VAL A 212      14.970 -19.802  27.762  1.00 57.99 C
ATOM   1658  CG2 VAL A 212      13.665 -18.988  29.707  1.00 65.40 C
ATOM   1659  N   THR A 213      11.738 -17.438  27.672  1.00 48.53 N
ATOM   1660  CA  THR A 213      11.698 -16.079  27.171  1.00 50.94 C
ATOM   1661  C   THR A 213      12.279 -15.100  28.194  1.00 46.89 C
ATOM   1662  O   THR A 213      11.760 -14.969  29.301  1.00 48.85 O
ATOM   1663  CB  THR A 213      10.246 -15.669  26.820  1.00 50.59 C
ATOM   1664  OG1 THR A 213       9.720 -16.556  25.827  1.00 54.06 O
ATOM   1665  CG2 THR A 213      10.214 -14.255  26.276  1.00 56.06 C
ATOM   1666  N   LEU A 214      13.367 -14.430  27.823  1.00 50.67 N
ATOM   1667  CA  LEU A 214      14.015 -13.445  28.686  1.00 44.75 C
ATOM   1668  C   LEU A 214      13.444 -12.078  28.327  1.00 49.46 C
ATOM   1669  O   LEU A 214      13.339 -11.738  27.147  1.00 40.16 O
ATOM   1670  CB  LEU A 214      15.519 -13.469  28.464  1.00 40.05 C
ATOM   1671  CG  LEU A 214      16.140 -14.857  28.611  1.00 47.06 C
ATOM   1672  CD1 LEU A 214      17.647 -14.728  28.666  1.00 41.62 C
ATOM   1673  CD2 LEU A 214      15.623 -15.532  29.880  1.00 42.47 C
ATOM   1674  N   VAL A 215      13.089 -11.299  29.345  1.00 44.86 N
ATOM   1675  CA  VAL A 215      12.454 -10.004  29.143  1.00 46.92 C
ATOM   1676  C   VAL A 215      13.030  -8.850  29.928  1.00 48.90 C
ATOM   1677  O   VAL A 215      13.254  -8.937  31.135  1.00 50.91 O
ATOM   1678  CB  VAL A 215      10.969 -10.089  29.508  1.00 49.64 C
ATOM   1679  CG1 VAL A 215      10.265  -8.759  29.213  1.00 50.90 C
ATOM   1680  CG2 VAL A 215      10.332 -11.234  28.765  1.00 52.37 C
ATOM   1681  N   CYS A 216      13.254  -7.755  29.221  1.00 44.39 N
ATOM   1682  CA  CYS A 216      13.754  -6.542  29.826  1.00 45.29 C
ATOM   1683  C   CYS A 216      12.744  -5.449  29.501  1.00 52.26 C
ATOM   1684  O   CYS A 216      12.223  -5.399  28.393  1.00 47.28 O
ATOM   1685  CB  CYS A 216      15.122  -6.180  29.257  1.00 45.92 C
ATOM   1686  SG  CYS A 216      16.483  -7.140  29.998  1.00 51.48 S
ATOM   1687  N   ASP A 217      12.454  -4.598  30.478  1.00 44.49 N
ATOM   1688  CA  ASP A 217      11.523  -3.499  30.291  1.00 46.18 C
ATOM   1689  C   ASP A 217      12.330  -2.230  30.313  1.00 46.02 C
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Figure 2 (Table 2 (page 38))

ATOM	1690	O	ASP	A	217	12.974	-1.906	31.307	1.00	42.34 O
ATOM	1691	CB	ASP	A	217	10.501	-3.453	31.419	1.00	43.07 C
ATOM	1692	CG	ASP	A	217	9.576	-4.624	31.382	1.00	54.67 C
ATOM	1693	OD1	ASP	A	217	8.860	-4.755	30.366	1.00	54.44 O
ATOM	1694	OD2	ASP	A	217	9.573	-5.417	32.350	1.00	52.78 O
ATOM	1695	N	ALA	A	218	12.279	-1.498	29.215	1.00	43.43 N
ATOM	1696	CA	ALA	A	218	13.030	-0.269	29.129	1.00	51.56 C
ATOM	1697	C	ALA	A	218	12.205	0.900	28.633	1.00	51.78 C
ATOM	1698	O	ALA	A	218	11.150	0.731	28.031	1.00	48.04 O
ATOM	1699	CB	ALA	A	218	14.221	-0.468	28.202	1.00	46.61 C
ATOM	1700	N	ASP	A	219	12.704	2.096	28.901	1.00	47.98 N
ATOM	1701	CA	ASP	A	219	12.076	3.287	28.377	1.00	53.40 C
ATOM	1702	C	ASP	A	219	13.097	4.412	28.287	1.00	54.39 C
ATOM	1703	O	ASP	A	219	14.214	4.308	28.791	1.00	53.10 O
ATOM	1704	CB	ASP	A	219	10.876	3.693	29.214	1.00	67.27 C
ATOM	1705	CG	ASP	A	219	11.226	3.878	30.644	1.00	73.00 C
ATOM	1706	OD1	ASP	A	219	12.424	4.087	30.905	1.00	77.65 O
ATOM	1707	OD2	ASP	A	219	10.315	3.824	31.502	1.00	83.21 O
ATOM	1708	N	GLY	A	220	12.693	5.482	27.622	1.00	46.12 N
ATOM	1709	CA	GLY	A	220	13.541	6.632	27.405	1.00	43.59 C
ATOM	1710	C	GLY	A	220	13.035	7.286	26.135	1.00	46.49 C
ATOM	1711	O	GLY	A	220	12.062	6.810	25.554	1.00	45.48 O
ATOM	1712	N	PHE	A	221	13.700	8.341	25.678	1.00	43.50 N
ATOM	1713	CA	PHE	A	221	13.283	9.017	24.465	1.00	42.29 C
ATOM	1714	C	PHE	A	221	14.499	9.499	23.669	1.00	33.90 C
ATOM	1715	O	PHE	A	221	15.313	10.265	24.178	1.00	43.58 O
ATOM	1716	CB	PHE	A	221	12.391	10.215	24.797	1.00	41.04 C
ATOM	1717	CG	PHE	A	221	11.792	10.861	23.572	1.00	44.52 C
ATOM	1718	CD1	PHE	A	221	10.591	10.395	23.037	1.00	47.33 C
ATOM	1719	CD2	PHE	A	221	12.482	11.863	22.891	1.00	44.34 C
ATOM	1720	CE1	PHE	A	221	10.088	10.910	21.837	1.00	45.26 C
ATOM	1721	CE2	PHE	A	221	11.989	12.380	21.693	1.00	48.97 C
ATOM	1722	CZ	PHE	A	221	10.785	11.897	21.166	1.00	44.61 C
ATOM	1723	N	PRO	A	222	14.645	9.050	22.400	1.00	40.11 N
ATOM	1724	CA	PRO	A	222	13.780	8.122	21.655	1.00	40.06 C
ATOM	1725	C	PRO	A	222	13.693	6.765	22.344	1.00	50.45 C
ATOM	1726	O	PRO	A	222	14.546	6.419	23.172	1.00	43.37 O
ATOM	1727	CB	PRO	A	222	14.480	8.000	20.307	1.00	44.90 C
ATOM	1728	CG	PRO	A	222	15.163	9.311	20.158	1.00	43.89 C
ATOM	1729	CD	PRO	A	222	15.733	9.547	21.536	1.00	38.16 C
ATOM	1730	N	GLU	A	223	12.659	5.999	21.998	1.00	47.32 N
ATOM	1731	CA	GLU	A	223	12.466	4.664	22.565	1.00	48.48 C
ATOM	1732	C	GLU	A	223	13.778	3.917	22.403	1.00	44.89 C
ATOM	1733	O	GLU	A	223	14.364	3.886	21.321	1.00	42.04 O
ATOM	1734	CB	GLU	A	223	11.359	3.905	21.837	1.00	51.24 C
ATOM	1735	CG	GLU	A	223	9.947	4.402	22.100	1.00	45.06 C
ATOM	1736	CD	GLU	A	223	9.513	4.303	23.556	1.00	60.54 C
ATOM	1737	OE1	GLU	A	223	9.950	3.368	24.263	1.00	71.83 O
ATOM	1738	OE2	GLU	A	223	8.700	5.153	23.986	1.00	70.97 O
ATOM	1739	N	PRO	A	224	14.249	3.296	23.483	1.00	46.34 N
ATOM	1740	CA	PRO	A	224	15.507	2.559	23.453	1.00	48.92 C
ATOM	1741	C	PRO	A	224	15.536	1.373	22.501	1.00	49.30 C
ATOM	1742	O	PRO	A	224	14.535	0.692	22.311	1.00	47.42 O
ATOM	1743	CB	PRO	A	224	15.678	2.113	24.911	1.00	47.68 C
ATOM	1744	CG	PRO	A	224	14.893	3.128	25.698	1.00	57.81 C
ATOM	1745	CD	PRO	A	224	13.673	3.314	24.843	1.00	47.48 C

Figure 2 (Table 2 (page 39))

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ATOM   1746  N   THR A 225      16.685   1.143  21.884  1.00 50.13 N
ATOM   1747  CA  THR A 225      16.859  -0.016  21.021  1.00 60.61 C
ATOM   1748  C   THR A 225      17.598  -1.033  21.907  1.00 59.15 C
ATOM   1749  O   THR A 225      18.533  -0.663  22.631  1.00 47.10 O
ATOM   1750  CB  THR A 225      17.723   0.319  19.810  1.00 58.08 C
ATOM   1751  OG1 THR A 225      17.027   1.259  18.985  1.00 83.82 O
ATOM   1752  CG2 THR A 225      18.009  -0.934  19.003  1.00 73.24 C
ATOM   1753  N   MET A 226      17.189  -2.296  21.862  1.00 52.21 N
ATOM   1754  CA  MET A 226      17.824  -3.310  22.692  1.00 53.46 C
ATOM   1755  C   MET A 226      18.721  -4.265  21.927  1.00 56.38 C
ATOM   1756  O   MET A 226      18.417  -4.657  20.802  1.00 51.69 O
ATOM   1757  CB  MET A 226      16.766  -4.149  23.397  1.00 61.02 C
ATOM   1758  CG  MET A 226      15.711  -3.339  24.112  1.00 73.13 C
ATOM   1759  SD  MET A 226      16.515  -2.409  25.388  1.00 79.72 S
ATOM   1760  CE  MET A 226      17.052  -3.791  26.474  1.00 72.80 C
ATOM   1761  N   SER A 227      19.821  -4.649  22.564  1.00 51.74 N
ATOM   1762  CA  SER A 227      20.755  -5.617  22.003  1.00 57.86 C
ATOM   1763  C   SER A 227      21.169  -6.496  23.187  1.00 61.93 C
ATOM   1764  O   SER A 227      21.204  -6.024  24.332  1.00 60.05 O
ATOM   1765  CB  SER A 227      21.961  -4.912  21.403  1.00 41.57 C
ATOM   1766  OG  SER A 227      22.546  -4.056  22.355  1.00 62.88 O
ATOM   1767  N   TRP A 228      21.472  -7.765  22.924  1.00 57.15 N
ATOM   1768  CA  TRP A 228      21.840  -8.689  23.998  1.00 55.47 C
ATOM   1769  C   TRP A 228      23.243  -9.290  23.899  1.00 59.04 C
ATOM   1770  O   TRP A 228      23.856  -9.273  22.829  1.00 49.40 O
ATOM   1771  CB  TRP A 228      20.842  -9.840  24.050  1.00 49.35 C
ATOM   1772  CG  TRP A 228      19.435  -9.439  24.308  1.00 47.96 C
ATOM   1773  CD1 TRP A 228      18.630  -8.695  23.494  1.00 53.38 C
ATOM   1774  CD2 TRP A 228      18.654  -9.760  25.462  1.00 47.76 C
ATOM   1775  NE1 TRP A 228      17.394  -8.537  24.067  1.00 52.08 N
ATOM   1776  CE2 TRP A 228      17.379  -9.177  25.279  1.00 45.77 C
ATOM   1777  CE3 TRP A 228      18.906 -10.482  26.637  1.00 42.71 C
ATOM   1778  CZ2 TRP A 228      16.355  -9.291  26.227  1.00 37.55 C
ATOM   1779  CZ3 TRP A 228      17.887 -10.598  27.586  1.00 45.83 C
ATOM   1780  CH2 TRP A 228      16.625 -10.004  27.373  1.00 50.85 C
ATOM   1781  N   THR A 229      23.749  -9.795  25.027  1.00 58.07 N
ATOM   1782  CA  THR A 229      25.047 -10.474  25.057  1.00 60.10 C
ATOM   1783  C   THR A 229      24.918 -11.741  25.902  1.00 61.83 C
ATOM   1784  O   THR A 229      24.132 -11.787  26.868  1.00 54.86 O
ATOM   1785  CB  THR A 229      26.191  -9.610  25.652  1.00 53.98 C
ATOM   1786  OG1 THR A 229      25.882  -9.252  26.999  1.00 57.01 O
ATOM   1787  CG2 THR A 229      26.418  -8.373  24.816  1.00 57.89 C
ATOM   1788  N   LYS A 230      25.677 -12.765  25.515  1.00 58.82 N
ATOM   1789  CA  LYS A 230      25.684 -14.043  26.217  1.00 58.37 C
ATOM   1790  C   LYS A 230      27.088 -14.147  26.792  1.00 52.83 C
ATOM   1791  O   LYS A 230      28.066 -14.266  26.054  1.00 54.49 O
ATOM   1792  CB  LYS A 230      25.396 -15.173  25.227  1.00 55.01 C
ATOM   1793  CG  LYS A 230      25.113 -16.539  25.849  1.00 45.56 C
ATOM   1794  CD  LYS A 230      24.973 -17.615  24.757  1.00 59.41 C
ATOM   1795  CE  LYS A 230      24.803 -19.019  25.339  1.00 62.34 C
ATOM   1796  NZ  LYS A 230      24.460 -20.050  24.304  1.00 59.23 N
ATOM   1797  N   ASP A 231      27.183 -14.078  28.115  1.00 61.62 N
ATOM   1798  CA  ASP A 231      28.479 -14.105  28.781  1.00 69.33 C
ATOM   1799  C   ASP A 231      29.439 -13.118  28.113  1.00 69.66 C
ATOM   1800  O   ASP A 231      30.612 -13.429  27.916  1.00 73.37 O
ATOM   1801  CB  ASP A 231      29.096 -15.509  28.754  1.00 67.95 C
```

Figure 2 (Table 2 (page 40))

```
ATOM   1802  CG  ASP A 231      28.359 -16.492  29.645  1.00 76.63 C
ATOM   1803  OD1 ASP A 231      27.830 -16.069  30.697  1.00 73.37 O
ATOM   1804  OD2 ASP A 231      28.327 -17.692  29.295  1.00 73.07 O
ATOM   1805  N   GLY A 232      28.939 -11.933  27.766  1.00 69.81 N
ATOM   1806  CA  GLY A 232      29.780 -10.925  27.147  1.00 62.92 C
ATOM   1807  C   GLY A 232      29.815 -10.953  25.633  1.00 57.21 C
ATOM   1808  O   GLY A 232      30.217  -9.985  24.999  1.00 64.11 O
ATOM   1809  N   GLU A 233      29.398 -12.058  25.039  1.00 60.24 N
ATOM   1810  CA  GLU A 233      29.407 -12.163  23.587  1.00 67.77 C
ATOM   1811  C   GLU A 233      28.086 -11.753  22.977  1.00 69.76 C
ATOM   1812  O   GLU A 233      27.019 -12.146  23.437  1.00 67.85 O
ATOM   1813  CB  GLU A 233      29.721 -13.589  23.156  1.00 73.47 C
ATOM   1814  CG  GLU A 233      31.174 -13.980  23.298  1.00 93.05 C
ATOM   1815  CD  GLU A 233      32.100 -13.154  22.416  1.00101.69 C
ATOM   1816  OE1 GLU A 233      31.753 -12.894  21.241  1.00104.10 O
ATOM   1817  OE2 GLU A 233      33.189 -12.771  22.898  1.00105.15 O
ATOM   1818  N   PRO A 234      28.146 -10.986  21.894  1.00 69.71 N
ATOM   1819  CA  PRO A 234      26.928 -10.527  21.227  1.00 69.07 C
ATOM   1820  C   PRO A 234      26.042 -11.660  20.747  1.00 63.95 C
ATOM   1821  O   PRO A 234      26.516 -12.774  20.513  1.00 68.33 O
ATOM   1822  CB  PRO A 234      27.463  -9.717  20.047  1.00 74.23 C
ATOM   1823  CG  PRO A 234      28.863  -9.346  20.458  1.00 78.24 C
ATOM   1824  CD  PRO A 234      29.349 -10.575  21.151  1.00 73.22 C
ATOM   1825  N   ILE A 235      24.756 -11.361  20.589  1.00 60.42 N
ATOM   1826  CA  ILE A 235      23.819 -12.347  20.075  1.00 59.30 C
ATOM   1827  C   ILE A 235      23.091 -11.707  18.887  1.00 73.94 C
ATOM   1828  O   ILE A 235      22.292 -10.780  19.062  1.00 69.18 O
ATOM   1829  CB  ILE A 235      22.785 -12.748  21.118  1.00 58.75 C
ATOM   1830  CG1 ILE A 235      23.480 -13.103  22.435  1.00 60.61 C
ATOM   1831  CG2 ILE A 235      21.986 -13.935  20.602  1.00 54.52 C
ATOM   1832  CD1 ILE A 235      22.535 -13.237  23.598  1.00 58.31 C
ATOM   1833  N   GLU A 236      23.341 -12.205  17.679  1.00 80.94 N
ATOM   1834  CA  GLU A 236      22.742 -11.605  16.488  1.00 90.13 C
ATOM   1835  C   GLU A 236      21.234 -11.755  16.308  1.00 93.13 C
ATOM   1836  O   GLU A 236      20.685 -12.857  16.339  1.00 89.58 O
ATOM   1837  CB  GLU A 236      23.493 -12.094  15.252  1.00 98.19 C
ATOM   1838  CG  GLU A 236      25.017 -12.039  15.429  1.00107.77 C
ATOM   1839  CD  GLU A 236      25.542 -10.662  15.844  1.00115.02 C
ATOM   1840  OE1 GLU A 236      24.988 -10.055  16.788  1.00121.81 O
ATOM   1841  OE2 GLU A 236      26.526 -10.191  15.233  1.00116.63 O
ATOM   1842  N   ASN A 237      20.585 -10.606  16.115  1.00 98.73 N
ATOM   1843  CA  ASN A 237      19.136 -10.494  15.944  1.00104.56 C
ATOM   1844  C   ASN A 237      18.609 -11.196  14.686  1.00110.81 C
ATOM   1845  O   ASN A 237      17.530 -11.792  14.705  1.00112.81 O
ATOM   1846  CB  ASN A 237      18.759  -9.004  15.930  1.00100.46 C
ATOM   1847  CG  ASN A 237      17.268  -8.761  16.142  1.00100.48 C
ATOM   1848  OD1 ASN A 237      16.868  -7.689  16.600  1.00 96.36 O
ATOM   1849  ND2 ASN A 237      16.443  -9.747  15.798  1.00 97.08 N
ATOM   1850  N   GLU A 238      19.382 -11.111  13.607  1.00114.86 N
ATOM   1851  CA  GLU A 238      19.072 -11.709  12.303  1.00120.04 C
ATOM   1852  C   GLU A 238      17.688 -12.328  12.095  1.00121.21 C
ATOM   1853  O   GLU A 238      16.975 -11.855  11.181  1.00121.72 O
ATOM   1854  CB  GLU A 238      20.152 -12.736  11.963  1.00121.17 C
ATOM   1855  CG  GLU A 238      21.557 -12.228  12.238  1.00126.14 C
ATOM   1856  CD  GLU A 238      21.808 -10.840  11.662  1.00130.48 C
ATOM   1857  OE1 GLU A 238      21.090  -9.885  12.034  1.00132.56 O
```

Figure 2 (Table 2 (page 41))

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ATOM   1858  OE2 GLU A 238      22.731 -10.705  10.837  1.00134.55 O
ATOM   1859  N   ASP A 241      18.070 -14.713   9.305  1.00127.03 N
ATOM   1860  CA  ASP A 241      17.685 -16.080   9.767  1.00127.98 C
ATOM   1861  C   ASP A 241      17.960 -16.274  11.255  1.00129.18 C
ATOM   1862  O   ASP A 241      18.938 -15.754  11.803  1.00129.01 O
ATOM   1863  CB  ASP A 241      18.443 -17.152   8.972  1.00124.42 C
ATOM   1864  CG  ASP A 241      18.044 -18.574   9.365  1.00123.20 C
ATOM   1865  OD1 ASP A 241      18.114 -18.916  10.570  1.00119.17 O
ATOM   1866  OD2 ASP A 241      17.664 -19.356   8.464  1.00120.27 O
ATOM   1867  N   ASP A 242      17.080 -17.043  11.888  1.00129.87 N
ATOM   1868  CA  ASP A 242      17.157 -17.357  13.310  1.00128.52 C
ATOM   1869  C   ASP A 242      16.420 -18.676  13.544  1.00124.12 C
ATOM   1870  O   ASP A 242      15.291 -18.851  13.081  1.00127.28 O
ATOM   1871  CB  ASP A 242      16.509 -16.230  14.128  1.00134.37 C
ATOM   1872  CG  ASP A 242      15.076 -15.931  13.693  1.00137.89 C
ATOM   1873  OD1 ASP A 242      14.695 -16.306  12.560  1.00139.91 O
ATOM   1874  OD2 ASP A 242      14.335 -15.302  14.484  1.00138.48 O
ATOM   1875  N   GLU A 243      17.053 -19.614  14.237  1.00115.47 N
ATOM   1876  CA  GLU A 243      16.401 -20.892  14.492  1.00108.81 C
ATOM   1877  C   GLU A 243      16.219 -21.065  15.984  1.00101.77 C
ATOM   1878  O   GLU A 243      15.232 -21.637  16.453  1.00 97.50 O
ATOM   1879  CB  GLU A 243      17.243 -22.056  13.957  1.00113.03 C
ATOM   1880  CG  GLU A 243      18.587 -22.269  14.665  1.00119.77 C
ATOM   1881  CD  GLU A 243      19.736 -21.500  14.022  1.00123.96 C
ATOM   1882  OE1 GLU A 243      20.004 -21.723  12.821  1.00128.49 O
ATOM   1883  OE2 GLU A 243      20.380 -20.682  14.716  1.00125.21 O
ATOM   1884  N   LYS A 244      17.193 -20.552  16.719  1.00 90.55 N
ATOM   1885  CA  LYS A 244      17.196 -20.652  18.159  1.00 87.36 C
ATOM   1886  C   LYS A 244      16.847 -19.342  18.851  1.00 78.94 C
ATOM   1887  O   LYS A 244      15.944 -19.299  19.681  1.00 79.48 O
ATOM   1888  CB  LYS A 244      18.567 -21.157  18.623  1.00 85.94 C
ATOM   1889  CG  LYS A 244      18.973 -20.687  20.009  1.00 90.77 C
ATOM   1890  CD  LYS A 244      20.222 -21.392  20.527  1.00 85.35 C
ATOM   1891  CE  LYS A 244      19.960 -22.872  20.764  1.00 85.15 C
ATOM   1892  NZ  LYS A 244      18.698 -23.096  21.533  1.00 79.01 N
ATOM   1893  N   HIS A 245      17.566 -18.279  18.510  1.00 72.67 N
ATOM   1894  CA  HIS A 245      17.332 -16.978  19.121  1.00 73.65 C
ATOM   1895  C   HIS A 245      16.275 -16.150  18.398  1.00 71.43 C
ATOM   1896  O   HIS A 245      16.483 -15.726  17.264  1.00 73.85 O
ATOM   1897  CB  HIS A 245      18.636 -16.191  19.174  1.00 62.45 C
ATOM   1898  CG  HIS A 245      19.712 -16.860  19.968  1.00 73.56 C
ATOM   1899  ND1 HIS A 245      19.566 -17.183  21.301  1.00 75.57 N
ATOM   1900  CD2 HIS A 245      20.963 -17.251  19.624  1.00 74.25 C
ATOM   1901  CE1 HIS A 245      20.680 -17.740  21.742  1.00 69.91 C
ATOM   1902  NE2 HIS A 245      21.542 -17.792  20.747  1.00 78.21 N
ATOM   1903  N   ILE A 246      15.151 -15.907  19.066  1.00 71.28 N
ATOM   1904  CA  ILE A 246      14.061 -15.117  18.492  1.00 67.47 C
ATOM   1905  C   ILE A 246      13.820 -13.823  19.279  1.00 68.54 C
ATOM   1906  O   ILE A 246      13.465 -13.871  20.459  1.00 56.11 O
ATOM   1907  CB  ILE A 246      12.746 -15.912  18.494  1.00 71.39 C
ATOM   1908  CG1 ILE A 246      12.953 -17.270  17.829  1.00 73.66 C
ATOM   1909  CG2 ILE A 246      11.656 -15.114  17.803  1.00 69.42 C
ATOM   1910  CD1 ILE A 246      13.544 -17.182  16.451  1.00 82.71 C
ATOM   1911  N   PHE A 247      13.991 -12.675  18.625  1.00 57.64 N
ATOM   1912  CA  PHE A 247      13.783 -11.395  19.286  1.00 57.66 C
ATOM   1913  C   PHE A 247      12.444 -10.766  19.000  1.00 59.75 C
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Figure 2 (Table 2 (page 42))

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ATOM   1914  O   PHE A 247      11.842 -11.003  17.955  1.00 71.91 O
ATOM   1915  CB  PHE A 247      14.831 -10.386  18.866  1.00 58.61 C
ATOM   1916  CG  PHE A 247      16.205 -10.761  19.252  1.00 55.18 C
ATOM   1917  CD1 PHE A 247      16.931 -11.663  18.486  1.00 63.52 C
ATOM   1918  CD2 PHE A 247      16.791 -10.195  20.375  1.00 64.94 C
ATOM   1919  CE1 PHE A 247      18.233 -11.994  18.836  1.00 56.98 C
ATOM   1920  CE2 PHE A 247      18.084 -10.515  20.735  1.00 62.89 C
ATOM   1921  CZ  PHE A 247      18.813 -11.416  19.963  1.00 69.14 C
ATOM   1922  N   SER A 248      11.984  -9.948  19.939  1.00 60.62 N
ATOM   1923  CA  SER A 248      10.741  -9.211  19.761  1.00 59.42 C
ATOM   1924  C   SER A 248      11.135  -8.035  18.848  1.00 58.07 C
ATOM   1925  O   SER A 248      12.324  -7.793  18.605  1.00 50.63 O
ATOM   1926  CB  SER A 248      10.238  -8.684  21.107  1.00 51.67 C
ATOM   1927  OG  SER A 248      11.212  -7.849  21.713  1.00 56.47 O
ATOM   1928  N   ASP A 249      10.156  -7.286  18.364  1.00 62.87 N
ATOM   1929  CA  ASP A 249      10.433  -6.168  17.461  1.00 68.58 C
ATOM   1930  C   ASP A 249      11.414  -5.157  18.016  1.00 71.42 C
ATOM   1931  O   ASP A 249      12.289  -4.649  17.304  1.00 70.32 O
ATOM   1932  CB  ASP A 249       9.113  -5.519  17.102  1.00 78.97 C
ATOM   1933  CG  ASP A 249       8.122  -6.538  16.598  1.00 85.41 C
ATOM   1934  OD1 ASP A 249       8.266  -6.986  15.438  1.00 90.50 O
ATOM   1935  OD2 ASP A 249       7.218  -6.926  17.370  1.00 85.77 O
ATOM   1936  N   ASP A 250      11.274  -4.875  19.297  1.00 71.27 N
ATOM   1937  CA  ASP A 250      12.159  -3.942  19.964  1.00 74.17 C
ATOM   1938  C   ASP A 250      13.358  -4.713  20.521  1.00 70.10 C
ATOM   1939  O   ASP A 250      14.337  -4.113  20.971  1.00 70.84 O
ATOM   1940  CB  ASP A 250      11.390  -3.284  21.100  1.00 82.42 C
ATOM   1941  CG  ASP A 250      10.583  -4.296  21.895  1.00 86.25 C
ATOM   1942  OD1 ASP A 250      10.204  -5.350  21.328  1.00 87.71 O
ATOM   1943  OD2 ASP A 250      10.316  -4.044  23.082  1.00 99.42 O
ATOM   1944  N   SER A 251      13.266  -6.044  20.478  1.00 61.34 N
ATOM   1945  CA  SER A 251      14.301  -6.932  21.005  1.00 60.93 C
ATOM   1946  C   SER A 251      14.357  -6.787  22.529  1.00 55.43 C
ATOM   1947  O   SER A 251      15.398  -6.997  23.149  1.00 54.55 O
ATOM   1948  CB  SER A 251      15.667  -6.615  20.386  1.00 56.47 C
ATOM   1949  OG  SER A 251      15.608  -6.719  18.971  1.00 68.26 O
ATOM   1950  N   SER A 252      13.222  -6.419  23.120  1.00 44.12 N
ATOM   1951  CA  SER A 252      13.132  -6.262  24.565  1.00 54.67 C
ATOM   1952  C   SER A 252      12.961  -7.666  25.142  1.00 45.19 C
ATOM   1953  O   SER A 252      13.231  -7.900  26.321  1.00 45.23 O
ATOM   1954  CB  SER A 252      11.948  -5.359  24.957  1.00 50.26 C
ATOM   1955  OG  SER A 252      10.705  -6.019  24.785  1.00 68.26 O
ATOM   1956  N   GLU A 253      12.511  -8.586  24.288  1.00 39.14 N
ATOM   1957  CA  GLU A 253      12.351  -9.984  24.655  1.00 42.86 C
ATOM   1958  C   GLU A 253      13.245 -10.847  23.787  1.00 55.42 C
ATOM   1959  O   GLU A 253      13.322 -10.649  22.573  1.00 55.46 O
ATOM   1960  CB  GLU A 253      10.924 -10.475  24.459  1.00 46.35 C
ATOM   1961  CG  GLU A 253       9.898  -9.823  25.335  1.00 52.21 C
ATOM   1962  CD  GLU A 253       8.629 -10.640  25.406  1.00 55.68 C
ATOM   1963  OE1 GLU A 253       8.464 -11.550  24.569  1.00 60.84 O
ATOM   1964  OE2 GLU A 253       7.792 -10.370  26.296  1.00 63.61 O
ATOM   1965  N   LEU A 254      13.925 -11.798  24.423  1.00 49.11 N
ATOM   1966  CA  LEU A 254      14.793 -12.741  23.730  1.00 43.78 C
ATOM   1967  C   LEU A 254      14.260 -14.129  24.052  1.00 54.16 C
ATOM   1968  O   LEU A 254      14.179 -14.516  25.221  1.00 49.96 O
ATOM   1969  CB  LEU A 254      16.240 -12.617  24.212  1.00 48.13 C
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Figure 2 (Table 2 (page 43))

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ATOM   1970  CG  LEU A 254      17.132 -13.793  23.786  1.00 61.15 C
ATOM   1971  CD1 LEU A 254      17.129 -13.902  22.264  1.00 56.30 C
ATOM   1972  CD2 LEU A 254      18.561 -13.622  24.314  1.00 45.18 C
ATOM   1973  N   THR A 255      13.874 -14.873  23.024  1.00 52.09 N
ATOM   1974  CA  THR A 255      13.343 -16.214  23.233  1.00 55.30 C
ATOM   1975  C   THR A 255      14.371 -17.254  22.822  1.00 57.05 C
ATOM   1976  O   THR A 255      14.809 -17.279  21.677  1.00 56.25 O
ATOM   1977  CB  THR A 255      12.050 -16.444  22.419  1.00 62.05 C
ATOM   1978  OG1 THR A 255      10.999 -15.630  22.951  1.00 66.84 O
ATOM   1979  CG2 THR A 255      11.625 -17.908  22.491  1.00 69.28 C
ATOM   1980  N   ILE A 256      14.784 -18.085  23.774  1.00 57.59 N
ATOM   1981  CA  ILE A 256      15.740 -19.140  23.482  1.00 53.88 C
ATOM   1982  C   ILE A 256      14.863 -20.362  23.227  1.00 55.73 C
ATOM   1983  O   ILE A 256      14.031 -20.740  24.050  1.00 53.74 O
ATOM   1984  CB  ILE A 256      16.721 -19.325  24.635  1.00 60.39 C
ATOM   1985  CG1 ILE A 256      17.478 -18.003  24.865  1.00 49.75 C
ATOM   1986  CG2 ILE A 256      17.729 -20.408  24.263  1.00 67.76 C
ATOM   1987  CD1 ILE A 256      18.337 -17.959  26.113  1.00 52.15 C
ATOM   1988  N   ARG A 257      15.049 -20.980  22.070  1.00 60.13 N
ATOM   1989  CA  ARG A 257      14.153 -22.051  21.657  1.00 71.50 C
ATOM   1990  C   ARG A 257      14.176 -23.516  22.065  1.00 69.32 C
ATOM   1991  O   ARG A 257      13.160 -24.049  22.523  1.00 80.18 O
ATOM   1992  CB  ARG A 257      14.007 -21.955  20.148  1.00 74.93 C
ATOM   1993  CG  ARG A 257      13.281 -20.678  19.720  1.00 86.48 C
ATOM   1994  CD  ARG A 257      11.972 -21.046  19.067  1.00 94.98 C
ATOM   1995  NE  ARG A 257      12.243 -22.177  18.190  1.00102.55 N
ATOM   1996  CZ  ARG A 257      11.403 -23.175  17.936  1.00101.10 C
ATOM   1997  NH1 ARG A 257      10.194 -23.198  18.481  1.00 98.39 N
ATOM   1998  NH2 ARG A 257      11.805 -24.190  17.182  1.00 99.09 N
ATOM   1999  N   ASN A 258      15.287 -24.195  21.864  1.00 61.69 N
ATOM   2000  CA  ASN A 258      15.340 -25.602  22.253  1.00 64.49 C
ATOM   2001  C   ASN A 258      16.465 -25.618  23.247  1.00 62.07 C
ATOM   2002  O   ASN A 258      17.624 -25.892  22.925  1.00 55.85 O
ATOM   2003  CB  ASN A 258      15.636 -26.481  21.041  1.00 66.15 C
ATOM   2004  CG  ASN A 258      14.404 -26.716  20.191  1.00 68.75 C
ATOM   2005  OD1 ASN A 258      13.379 -27.234  20.673  1.00 64.25 O
ATOM   2006  ND2 ASN A 258      14.484 -26.329  18.926  1.00 70.00 N
ATOM   2007  N   VAL A 259      16.094 -25.272  24.468  1.00 62.90 N
ATOM   2008  CA  VAL A 259      17.049 -25.157  25.545  1.00 65.80 C
ATOM   2009  C   VAL A 259      17.876 -26.384  25.872  1.00 58.88 C
ATOM   2010  O   VAL A 259      17.365 -27.483  26.054  1.00 56.71 O
ATOM   2011  CB  VAL A 259      16.370 -24.703  26.858  1.00 64.49 C
ATOM   2012  CG1 VAL A 259      17.433 -24.328  27.883  1.00 63.04 C
ATOM   2013  CG2 VAL A 259      15.437 -23.546  26.599  1.00 62.50 C
ATOM   2014  N   ASP A 260      19.176 -26.159  25.951  1.00 60.37 N
ATOM   2015  CA  ASP A 260      20.110 -27.191  26.329  1.00 64.76 C
ATOM   2016  C   ASP A 260      21.141 -26.491  27.190  1.00 63.70 C
ATOM   2017  O   ASP A 260      21.185 -25.257  27.253  1.00 55.60 O
ATOM   2018  CB  ASP A 260      20.785 -27.829  25.120  1.00 61.25 C
ATOM   2019  CG  ASP A 260      21.602 -26.844  24.322  1.00 68.49 C
ATOM   2020  OD1 ASP A 260      22.091 -25.847  24.896  1.00 68.44 O
ATOM   2021  OD2 ASP A 260      21.775 -27.084  23.110  1.00 81.31 O
ATOM   2022  N   LYS A 261      21.986 -27.277  27.832  1.00 57.12 N
ATOM   2023  CA  LYS A 261      22.985 -26.711  28.711  1.00 51.64 C
ATOM   2024  C   LYS A 261      23.832 -25.591  28.141  1.00 46.97 C
ATOM   2025  O   LYS A 261      24.335 -24.757  28.895  1.00 48.66 O
```

Figure 2 (Table 2 (page 44))

```
ATOM   2026  CB  LYS A 261      23.874 -27.828  29.258  1.00 52.71 C
ATOM   2027  CG  LYS A 261      23.193 -28.612  30.358  1.00 61.87 C
ATOM   2028  CD  LYS A 261      24.105 -29.669  30.947  1.00 73.37 C
ATOM   2029  CE  LYS A 261      23.600 -30.117  32.308  1.00 76.85 C
ATOM   2030  NZ  LYS A 261      23.680 -29.007  33.304  1.00 77.99 N
ATOM   2031  N   ASN A 262      24.004 -25.534  26.827  1.00 51.62 N
ATOM   2032  CA  ASN A 262      24.834 -24.464  26.278  1.00 50.71 C
ATOM   2033  C   ASN A 262      24.189 -23.099  26.414  1.00 49.52 C
ATOM   2034  O   ASN A 262      24.835 -22.073  26.224  1.00 44.29 O
ATOM   2035  CB  ASN A 262      25.160 -24.707  24.815  1.00 63.69 C
ATOM   2036  CG  ASN A 262      26.545 -25.256  24.636  1.00 76.99 C
ATOM   2037  OD1 ASN A 262      27.466 -24.881  25.368  1.00 88.03 O
ATOM   2038  ND2 ASN A 262      26.713 -26.145  23.664  1.00 83.71 N
ATOM   2039  N   ASP A 263      22.911 -23.100  26.755  1.00 43.87 N
ATOM   2040  CA  ASP A 263      22.173 -21.864  26.915  1.00 49.29 C
ATOM   2041  C   ASP A 263      22.341 -21.257  28.307  1.00 56.55 C
ATOM   2042  O   ASP A 263      21.984 -20.103  28.532  1.00 45.77 O
ATOM   2043  CB  ASP A 263      20.705 -22.115  26.593  1.00 46.15 C
ATOM   2044  CG  ASP A 263      20.502 -22.558  25.148  1.00 47.16 C
ATOM   2045  OD1 ASP A 263      21.208 -22.006  24.272  1.00 50.06 O
ATOM   2046  OD2 ASP A 263      19.642 -23.440  24.894  1.00 53.96 O
ATOM   2047  N   GLU A 264      22.886 -22.033  29.241  1.00 52.20 N
ATOM   2048  CA  GLU A 264      23.126 -21.517  30.580  1.00 50.47 C
ATOM   2049  C   GLU A 264      24.217 -20.455  30.464  1.00 55.25 C
ATOM   2050  O   GLU A 264      25.286 -20.722  29.917  1.00 51.52 O
ATOM   2051  CB  GLU A 264      23.575 -22.644  31.526  1.00 49.18 C
ATOM   2052  CG  GLU A 264      23.865 -22.150  32.948  1.00 56.13 C
ATOM   2053  CD  GLU A 264      24.070 -23.270  33.968  1.00 59.96 C
ATOM   2054  OE1 GLU A 264      23.144 -24.088  34.166  1.00 52.27 O
ATOM   2055  OE2 GLU A 264      25.161 -23.319  34.575  1.00 63.96 O
ATOM   2056  N   ALA A 265      23.936 -19.254  30.971  1.00 50.58 N
ATOM   2057  CA  ALA A 265      24.882 -18.143  30.932  1.00 49.56 C
ATOM   2058  C   ALA A 265      24.285 -16.892  31.553  1.00 44.28 C
ATOM   2059  O   ALA A 265      23.138 -16.876  32.020  1.00 44.60 O
ATOM   2060  CB  ALA A 265      25.275 -17.839  29.485  1.00 55.17 C
ATOM   2061  N   GLU A 266      25.084 -15.837  31.565  1.00 46.95 N
ATOM   2062  CA  GLU A 266      24.597 -14.566  32.052  1.00 58.95 C
ATOM   2063  C   GLU A 266      24.233 -13.782  30.796  1.00 54.06 C
ATOM   2064  O   GLU A 266      25.077 -13.547  29.937  1.00 49.16 O
ATOM   2065  CB  GLU A 266      25.662 -13.784  32.824  1.00 49.59 C
ATOM   2066  CG  GLU A 266      25.188 -12.371  33.185  1.00 68.76 C
ATOM   2067  CD  GLU A 266      26.312 -11.461  33.655  1.00 79.04 C
ATOM   2068  OE1 GLU A 266      27.442 -11.585  33.135  1.00 92.30 O
ATOM   2069  OE2 GLU A 266      26.071 -10.604  34.534  1.00 84.00 O
ATOM   2070  N   TYR A 267      22.969 -13.405  30.682  1.00 56.50 N
ATOM   2071  CA  TYR A 267      22.539 -12.620  29.539  1.00 53.55 C
ATOM   2072  C   TYR A 267      22.379 -11.175  29.973  1.00 53.33 C
ATOM   2073  O   TYR A 267      21.857 -10.899  31.051  1.00 56.26 O
ATOM   2074  CB  TYR A 267      21.216 -13.131  29.000  1.00 41.05 C
ATOM   2075  CG  TYR A 267      21.302 -14.503  28.392  1.00 52.19 C
ATOM   2076  CD1 TYR A 267      21.310 -15.645  29.200  1.00 46.18 C
ATOM   2077  CD2 TYR A 267      21.374 -14.669  27.010  1.00 42.85 C
ATOM   2078  CE1 TYR A 267      21.385 -16.907  28.649  1.00 36.41 C
ATOM   2079  CE2 TYR A 267      21.447 -15.926  26.447  1.00 47.87 C
ATOM   2080  CZ  TYR A 267      21.454 -17.043  27.269  1.00 46.20 C
ATOM   2081  OH  TYR A 267      21.534 -18.289  26.709  1.00 46.42 O
```

Figure 2 (Table 2 (page 45))

```
ATOM   2082  N   VAL A 268      22.849 -10.259  29.134  1.00 54.55 N
ATOM   2083  CA  VAL A 268      22.744  -8.833  29.420  1.00 51.27 C
ATOM   2084  C   VAL A 268      21.939  -8.121  28.325  1.00 53.04 C
ATOM   2085  O   VAL A 268      22.238  -8.268  27.140  1.00 49.32 O
ATOM   2086  CB  VAL A 268      24.149  -8.164  29.507  1.00 51.72 C
ATOM   2087  CG1 VAL A 268      24.008  -6.653  29.697  1.00 53.25 C
ATOM   2088  CG2 VAL A 268      24.954  -8.757  30.667  1.00 53.72 C
ATOM   2089  N   CYS A 269      20.909  -7.372  28.708  1.00 47.02 N
ATOM   2090  CA  CYS A 269      20.130  -6.631  27.712  1.00 46.07 C
ATOM   2091  C   CYS A 269      20.572  -5.192  27.825  1.00 48.28 C
ATOM   2092  O   CYS A 269      20.513  -4.568  28.893  1.00 54.75 O
ATOM   2093  CB  CYS A 269      18.645  -6.725  27.972  1.00 47.89 C
ATOM   2094  SG  CYS A 269      18.154  -6.060  29.588  1.00 57.20 S
ATOM   2095  N   ILE A 270      21.040  -4.684  26.705  1.00 44.49 N
ATOM   2096  CA  ILE A 270      21.542  -3.334  26.618  1.00 54.21 C
ATOM   2097  C   ILE A 270      20.492  -2.429  25.984  1.00 51.98 C
ATOM   2098  O   ILE A 270      20.057  -2.665  24.858  1.00 52.39 O
ATOM   2099  CB  ILE A 270      22.804  -3.333  25.757  1.00 58.16 C
ATOM   2100  CG1 ILE A 270      23.777  -4.385  26.287  1.00 59.14 C
ATOM   2101  CG2 ILE A 270      23.451  -1.964  25.768  1.00 58.07 C
ATOM   2102  CD1 ILE A 270      24.907  -4.698  25.332  1.00 62.65 C
ATOM   2103  N   ALA A 271      20.068  -1.413  26.725  1.00 46.08 N
ATOM   2104  CA  ALA A 271      19.081  -0.463  26.220  1.00 43.82 C
ATOM   2105  C   ALA A 271      19.811   0.838  25.863  1.00 41.91 C
ATOM   2106  O   ALA A 271      20.461   1.454  26.713  1.00 41.51 O
ATOM   2107  CB  ALA A 271      18.010  -0.212  27.272  1.00 40.50 C
ATOM   2108  N   GLU A 272      19.709   1.242  24.601  1.00 43.98 N
ATOM   2109  CA  GLU A 272      20.375   2.453  24.128  1.00 50.40 C
ATOM   2110  C   GLU A 272      19.526   3.346  23.255  1.00 40.39 C
ATOM   2111  O   GLU A 272      18.635   2.880  22.548  1.00 43.66 O
ATOM   2112  CB  GLU A 272      21.589   2.115  23.251  1.00 46.89 C
ATOM   2113  CG  GLU A 272      22.738   1.366  23.863  1.00 76.32 C
ATOM   2114  CD  GLU A 272      23.835   1.101  22.832  1.00 88.35 C
ATOM   2115  OE1 GLU A 272      23.496   0.886  21.643  1.00 95.66 O
ATOM   2116  OE2 GLU A 272      25.031   1.096  23.206  1.00 91.47 O
ATOM   2117  N   ASN A 273      19.843   4.635  23.316  1.00 46.76 N
ATOM   2118  CA  ASN A 273      19.260   5.648  22.438  1.00 47.59 C
ATOM   2119  C   ASN A 273      20.335   6.718  22.340  1.00 52.11 C
ATOM   2120  O   ASN A 273      21.366   6.622  23.008  1.00 44.76 O
ATOM   2121  CB  ASN A 273      17.897   6.201  22.916  1.00 46.27 C
ATOM   2122  CG  ASN A 273      17.964   6.980  24.211  1.00 44.51 C
ATOM   2123  OD1 ASN A 273      19.012   7.471  24.611  1.00 44.37 O
ATOM   2124  ND2 ASN A 273      16.808   7.126  24.866  1.00 38.00 N
ATOM   2125  N   LYS A 274      20.128   7.723  21.504  1.00 56.80 N
ATOM   2126  CA  LYS A 274      21.154   8.740  21.317  1.00 51.83 C
ATOM   2127  C   LYS A 274      21.618   9.485  22.567  1.00 54.11 C
ATOM   2128  O   LYS A 274      22.667  10.123  22.545  1.00 58.51 O
ATOM   2129  CB  LYS A 274      20.718   9.742  20.238  1.00 55.02 C
ATOM   2130  CG  LYS A 274      19.590  10.658  20.644  1.00 47.96 C
ATOM   2131  CD  LYS A 274      18.892  11.218  19.403  1.00 52.54 C
ATOM   2132  CE  LYS A 274      19.784  12.175  18.622  1.00 65.50 C
ATOM   2133  NZ  LYS A 274      19.120  12.652  17.364  1.00 68.41 N
ATOM   2134  N   ALA A 275      20.869   9.403  23.659  1.00 47.65 N
ATOM   2135  CA  ALA A 275      21.275  10.100  24.868  1.00 48.41 C
ATOM   2136  C   ALA A 275      21.944   9.233  25.930  1.00 49.48 C
ATOM   2137  O   ALA A 275      22.294   9.735  26.988  1.00 50.34 O
```

Figure 2 (Table 2 (page 46))

```
ATOM   2138  CB  ALA A 275      20.084  10.814  25.487  1.00 44.55 C
ATOM   2139  N   GLY A 276      22.122   7.942  25.691  1.00 49.34 N
ATOM   2140  CA  GLY A 276      22.755   7.177  26.746  1.00 51.88 C
ATOM   2141  C   GLY A 276      22.482   5.694  26.738  1.00 50.21 C
ATOM   2142  O   GLY A 276      21.907   5.164  25.779  1.00 51.48 O
ATOM   2143  N   GLU A 277      22.868   5.026  27.824  1.00 50.99 N
ATOM   2144  CA  GLU A 277      22.696   3.586  27.906  1.00 53.05 C
ATOM   2145  C   GLU A 277      22.598   3.056  29.316  1.00 51.11 C
ATOM   2146  O   GLU A 277      23.116   3.655  30.249  1.00 52.32 O
ATOM   2147  CB  GLU A 277      23.873   2.915  27.194  1.00 58.98 C
ATOM   2148  CG  GLU A 277      23.900   1.389  27.218  1.00 74.31 C
ATOM   2149  CD  GLU A 277      24.570   0.797  28.462  1.00 89.46 C
ATOM   2150  OE1 GLU A 277      25.277   1.537  29.183  1.00 96.28 O
ATOM   2151  OE2 GLU A 277      24.398  -0.420  28.705  1.00 89.19 O
ATOM   2152  N   GLN A 278      21.907   1.927  29.453  1.00 49.66 N
ATOM   2153  CA  GLN A 278      21.783   1.228  30.724  1.00 45.13 C
ATOM   2154  C   GLN A 278      21.513  -0.239  30.415  1.00 50.42 C
ATOM   2155  O   GLN A 278      20.877  -0.568  29.417  1.00 46.75 O
ATOM   2156  CB  GLN A 278      20.662   1.789  31.607  1.00 48.09 C
ATOM   2157  CG  GLN A 278      20.812   1.327  33.064  1.00 46.69 C
ATOM   2158  CD  GLN A 278      19.700   1.822  33.976  1.00 57.97 C
ATOM   2159  OE1 GLN A 278      18.572   1.330  33.917  1.00 44.46 O
ATOM   2160  NE2 GLN A 278      20.012   2.800  34.826  1.00 53.33 N
ATOM   2161  N   ASP A 279      22.013  -1.132  31.257  1.00 45.92 N
ATOM   2162  CA  ASP A 279      21.795  -2.541  31.014  1.00 47.69 C
ATOM   2163  C   ASP A 279      21.345  -3.251  32.270  1.00 47.71 C
ATOM   2164  O   ASP A 279      21.357  -2.687  33.366  1.00 48.35 O
ATOM   2165  CB  ASP A 279      23.062  -3.186  30.451  1.00 60.02 C
ATOM   2166  CG  ASP A 279      24.316  -2.707  31.154  1.00 69.17 C
ATOM   2167  OD1 ASP A 279      24.456  -2.954  32.370  1.00 75.17 O
ATOM   2168  OD2 ASP A 279      25.157  -2.073  30.490  1.00 75.70 O
ATOM   2169  N   ALA A 280      20.892  -4.480  32.079  1.00 49.27 N
ATOM   2170  CA  ALA A 280      20.428  -5.314  33.172  1.00 57.28 C
ATOM   2171  C   ALA A 280      20.804  -6.748  32.833  1.00 54.10 C
ATOM   2172  O   ALA A 280      20.868  -7.126  31.659  1.00 47.63 O
ATOM   2173  CB  ALA A 280      18.909  -5.184  33.341  1.00 47.77 C
ATOM   2174  N   SER A 281      21.043  -7.560  33.854  1.00 53.68 N
ATOM   2175  CA  SER A 281      21.429  -8.931  33.599  1.00 48.69 C
ATOM   2176  C   SER A 281      20.402  -9.952  34.031  1.00 45.20 C
ATOM   2177  O   SER A 281      19.595  -9.718  34.934  1.00 45.89 O
ATOM   2178  CB  SER A 281      22.768  -9.219  34.279  1.00 61.38 C
ATOM   2179  OG  SER A 281      22.718  -8.863  35.646  1.00 57.59 O
ATOM   2180  N   ILE A 282      20.427 -11.086  33.349  1.00 43.38 N
ATOM   2181  CA  ILE A 282      19.524 -12.185  33.637  1.00 41.38 C
ATOM   2182  C   ILE A 282      20.392 -13.429  33.671  1.00 47.86 C
ATOM   2183  O   ILE A 282      21.235 -13.631  32.799  1.00 51.03 O
ATOM   2184  CB  ILE A 282      18.436 -12.316  32.548  1.00 40.14 C
ATOM   2185  CG1 ILE A 282      17.557 -11.056  32.557  1.00 46.94 C
ATOM   2186  CG2 ILE A 282      17.576 -13.549  32.807  1.00 42.53 C
ATOM   2187  CD1 ILE A 282      16.484 -10.998  31.476  1.00 45.40 C
ATOM   2188  N   HIS A 283      20.204 -14.248  34.695  1.00 45.39 N
ATOM   2189  CA  HIS A 283      20.998 -15.458  34.816  1.00 46.01 C
ATOM   2190  C   HIS A 283      20.145 -16.651  34.501  1.00 41.84 C
ATOM   2191  O   HIS A 283      19.164 -16.923  35.197  1.00 51.27 O
ATOM   2192  CB  HIS A 283      21.570 -15.575  36.230  1.00 53.96 C
ATOM   2193  CG  HIS A 283      22.617 -14.551  36.543  1.00 60.28 C
```

Figure 2 (Table 2 (page 47))

```
ATOM   2194  ND1 HIS A 283      23.908 -14.633  36.065  1.00 69.25 N
ATOM   2195  CD2 HIS A 283      22.554 -13.401  37.260  1.00 68.71 C
ATOM   2196  CE1 HIS A 283      24.593 -13.578  36.473  1.00 75.43 C
ATOM   2197  NE2 HIS A 283      23.796 -12.816  37.199  1.00 66.88 N
ATOM   2198  N   LEU A 284      20.499 -17.349  33.427  1.00 41.70 N
ATOM   2199  CA  LEU A 284      19.752 -18.534  33.050  1.00 45.86 C
ATOM   2200  C   LEU A 284      20.533 -19.778  33.469  1.00 49.53 C
ATOM   2201  O   LEU A 284      21.683 -19.963  33.058  1.00 45.44 O
ATOM   2202  CB  LEU A 284      19.515 -18.576  31.532  1.00 41.74 C
ATOM   2203  CG  LEU A 284      18.782 -19.827  31.028  1.00 47.91 C
ATOM   2204  CD1 LEU A 284      17.407 -19.888  31.680  1.00 45.59 C
ATOM   2205  CD2 LEU A 284      18.648 -19.810  29.500  1.00 48.70 C
ATOM   2206  N   LYS A 285      19.913 -20.625  34.285  1.00 48.59 N
ATOM   2207  CA  LYS A 285      20.557 -21.863  34.711  1.00 53.60 C
ATOM   2208  C   LYS A 285      19.797 -23.008  34.061  1.00 46.75 C
ATOM   2209  O   LYS A 285      18.570 -23.061  34.109  1.00 49.33 O
ATOM   2210  CB  LYS A 285      20.531 -21.991  36.239  1.00 56.58 C
ATOM   2211  CG  LYS A 285      21.302 -20.880  36.942  1.00 63.01 C
ATOM   2212  CD  LYS A 285      21.254 -21.021  38.459  1.00 71.05 C
ATOM   2213  CE  LYS A 285      21.853 -19.795  39.148  1.00 76.77 C
ATOM   2214  NZ  LYS A 285      20.993 -18.583  39.020  1.00 73.22 N
ATOM   2215  N   VAL A 286      20.525 -23.922  33.436  1.00 44.47 N
ATOM   2216  CA  VAL A 286      19.888 -25.047  32.759  1.00 53.73 C
ATOM   2217  C   VAL A 286      20.271 -26.367  33.410  1.00 58.55 C
ATOM   2218  O   VAL A 286      21.446 -26.709  33.489  1.00 58.02 O
ATOM   2219  CB  VAL A 286      20.283 -25.078  31.268  1.00 49.11 C
ATOM   2220  CG1 VAL A 286      19.618 -26.248  30.572  1.00 52.83 C
ATOM   2221  CG2 VAL A 286      19.872 -23.760  30.597  1.00 49.45 C
ATOM   2222  N   PHE A 287      19.267 -27.100  33.875  1.00 56.62 N
ATOM   2223  CA  PHE A 287      19.493 -28.379  34.528  1.00 60.81 C
ATOM   2224  C   PHE A 287      19.172 -29.540  33.607  1.00 64.78 C
ATOM   2225  O   PHE A 287      18.208 -29.487  32.846  1.00 64.16 O
ATOM   2226  CB  PHE A 287      18.645 -28.461  35.795  1.00 58.95 C
ATOM   2227  CG  PHE A 287      18.868 -27.314  36.724  1.00 61.24 C
ATOM   2228  CD1 PHE A 287      17.963 -26.259  36.783  1.00 56.19 C
ATOM   2229  CD2 PHE A 287      20.036 -27.237  37.477  1.00 62.69 C
ATOM   2230  CE1 PHE A 287      18.224 -25.139  37.575  1.00 53.03 C
ATOM   2231  CE2 PHE A 287      20.304 -26.124  38.266  1.00 58.31 C
ATOM   2232  CZ  PHE A 287      19.397 -25.073  38.314  1.00 59.07 C
ATOM   2233  N   ALA A 288      19.997 -30.583  33.666  1.00 66.33 N
ATOM   2234  CA  ALA A 288      19.795 -31.766  32.834  1.00 73.18 C
ATOM   2235  C   ALA A 288      18.428 -32.377  33.119  1.00 78.08 C
ATOM   2236  O   ALA A 288      17.960 -32.349  34.259  1.00 78.39 O
ATOM   2237  CB  ALA A 288      20.887 -32.785  33.106  1.00 69.96 C
ATOM   2238  N   LYS A 289      17.794 -32.931  32.087  1.00 80.55 N
ATOM   2239  CA  LYS A 289      16.476 -33.541  32.240  1.00 84.08 C
ATOM   2240  C   LYS A 289      16.535 -34.855  33.016  1.00 88.56 C
ATOM   2241  O   LYS A 289      15.585 -35.127  33.785  1.00 92.60 O
ATOM   2242  CB  LYS A 289      15.830 -33.779  30.872  1.00 82.11 C
ATOM   2243  CG  LYS A 289      16.538 -34.804  30.009  1.00 82.83 C
ATOM   2244  CD  LYS A 289      15.739 -35.066  28.748  1.00 81.13 C
ATOM   2245  CE  LYS A 289      16.362 -36.164  27.910  1.00 87.98 C
ATOM   2246  NZ  LYS A 289      15.562 -36.424  26.677  1.00 90.82 N
ATOM   2247  OXT LYS A 289      17.519 -35.608  32.835  1.00 94.14 O
TER    2248      LYS A 289
HETATM 2249  O   HOH     1      26.862  53.829  -2.499  1.00 53.80 O
```

Figure 2 (Table 2 (page 48))

HETATM	2250	O	HOH	2	31.435	56.206	-5.661	1.00	53.53 O
HETATM	2251	O	HOH	4	18.815	60.633	-12.908	1.00	43.98 O
HETATM	2252	O	HOH	5	16.291	34.157	5.585	1.00	64.41 O
HETATM	2253	O	HOH	6	24.283	23.825	11.233	1.00	59.48 O
HETATM	2254	O	HOH	7	21.204	19.365	17.749	1.00	60.83 O
HETATM	2255	O	HOH	8	15.430	12.803	19.226	1.00	45.67 O
HETATM	2256	O	HOH	9	22.245	15.815	31.410	1.00	50.19 O
HETATM	2257	O	HOH	10	25.429	21.325	30.709	1.00	49.37 O
HETATM	2258	O	HOH	11	23.048	36.010	15.248	1.00	51.13 O
HETATM	2259	O	HOH	12	29.692	33.165	19.866	1.00	37.03 O
HETATM	2260	O	HOH	13	9.169	23.139	31.247	1.00	61.40 O
HETATM	2261	O	HOH	14	17.022	56.166	8.038	1.00	75.27 O
HETATM	2262	O	HOH	15	8.769	40.002	7.174	1.00	48.91 O
HETATM	2263	O	HOH	16	10.231	43.238	7.473	1.00	47.42 O
HETATM	2264	O	HOH	17	15.641	26.081	5.720	1.00	78.13 O
HETATM	2265	O	HOH	18	20.551	14.627	22.658	1.00	46.05 O
HETATM	2266	O	HOH	19	11.221	-2.472	26.804	1.00	52.85 O
HETATM	2267	O	HOH	20	13.041	60.224	-4.320	1.00	64.49 O
HETATM	2268	O	HOH	21	14.835	48.897	-2.048	1.00	85.96 O
HETATM	2269	O	HOH	22	29.546	51.498	-21.147	1.00	47.61 O
HETATM	2270	O	HOH	23	24.511	42.141	-28.698	1.00	76.55 O
HETATM	2271	O	HOH	25	21.636	45.365	-18.499	1.00	37.40 O
HETATM	2272	O	HOH	26	15.790	47.805	-19.728	1.00	64.11 O
HETATM	2273	O	HOH	27	20.999	58.533	-6.980	1.00	47.49 O
HETATM	2274	O	HOH	28	14.534	40.436	5.659	1.00	59.32 O
HETATM	2275	O	HOH	29	18.746	16.322	14.473	1.00	79.28 O
HETATM	2276	O	HOH	30	25.965	40.212	9.533	1.00	52.16 O
HETATM	2277	O	HOH	31	16.482	55.396	13.144	1.00	59.76 O
HETATM	2278	O	HOH	32	9.922	15.732	20.883	1.00	48.37 O
HETATM	2279	O	HOH	33	11.915	-0.137	41.445	1.00	73.91 O
HETATM	2280	O	HOH	34	11.044	7.531	19.815	1.00	49.89 O
HETATM	2281	O	HOH	35	6.902	3.742	25.922	1.00	63.36 O
HETATM	2282	O	HOH	37	21.399	-1.338	20.994	1.00	76.17 O
HETATM	2283	O	HOH	38	18.329	53.773	-1.977	1.00	62.61 O
HETATM	2284	O	HOH	39	18.014	43.718	-2.937	1.00	49.73 O
HETATM	2285	O	HOH	40	32.281	40.568	-12.177	1.00	66.60 O
HETATM	2286	O	HOH	41	19.381	44.469	-19.805	1.00	64.16 O
HETATM	2287	O	HOH	42	25.046	41.566	-20.577	1.00	61.50 O
HETATM	2288	O	HOH	46	7.104	2.690	28.661	1.00	90.82 O
HETATM	2289	O	HOH	48	29.774	-14.171	32.170	1.00	72.60 O
HETATM	2290	O	HOH	49	36.677	48.530	-18.261	1.00	57.32 O
HETATM	2291	O	HOH	50	33.317	46.204	-17.946	1.00	47.09 O
HETATM	2292	O	HOH	52	22.357	37.802	16.682	1.00	62.95 O
HETATM	2293	O	HOH	54	11.598	9.583	18.307	1.00	51.71 O
HETATM	2294	O	HOH	55	22.448	12.959	33.086	1.00	71.24 O
HETATM	2295	O	HOH	56	12.323	-25.457	30.778	1.00	69.54 O
HETATM	2296	O	HOH	57	22.080	16.779	21.536	1.00	49.07 O
HETATM	2297	O	HOH	58	17.068	4.212	19.556	1.00	71.54 O
HETATM	2298	O	HOH	59	21.824	23.695	19.290	1.00	44.38 O
HETATM	2299	O	HOH	60	17.965	7.263	19.831	1.00	45.41 O
HETATM	2300	O	HOH	61	19.593	-1.710	35.113	1.00	49.69 O
HETATM	2301	O	HOH	62	18.642	-7.793	36.955	1.00	68.54 O
HETATM	2302	O	HOH	63	23.848	-0.227	33.498	1.00	54.90 O
HETATM	2303	O	HOH	64	31.052	-17.541	34.986	1.00	68.80 O
HETATM	2304	O	HOH	65	5.551	-4.238	9.968	1.00	64.86 O
HETATM	2305	O	HOH	66	10.472	-3.423	9.588	1.00	81.77 O

Figure 2 (Table 2 (page 49))

```
HETATM 2306  O   HOH    67       6.705  -3.198  12.269  1.00 59.36 O
HETATM 2307  O   HOH    68      18.934   8.523  16.255  1.00 70.67 O
HETATM 2308  O   HOH    69      26.373 -11.223  28.910  1.00 53.04 O
HETATM 2309  O   HOH    70      26.631   6.184  27.729  1.00 74.30 O
HETATM 2310  O   HOH    71      26.466 -20.918  34.876  1.00 70.68 O
HETATM 2311  O   HOH    72       8.293  12.647  18.395  1.00 56.61 O
HETATM 2312  O   HOH    74      17.106  -5.693  36.496  1.00 48.96 O
HETATM 2313  O   HOH    75       1.311  -8.583   8.383  1.00 70.05 O
HETATM 2314  O   HOH    76      26.233  40.015   4.081  1.00 64.69 O
HETATM 2315  O   HOH    77      21.018  39.423   0.780  1.00 63.73 O
HETATM 2316  O   HOH    78      30.385  47.077  -9.984  1.00 47.01 O
HETATM 2317  O   HOH    80      17.757  22.465   9.580  1.00 54.37 O
HETATM 2318  O   HOH    81      25.847  39.446  18.635  1.00 61.83 O
HETATM 2319  O   HOH    82      23.903 -18.248  35.163  1.00 66.46 O
HETATM 2320  O   HOH    83      17.550  29.059   7.625  1.00 69.50 O
HETATM 2321  O   HOH    84      22.192  30.581  38.779  1.00 45.18 O
HETATM 2322  O   HOH    85      19.724  26.758   8.865  1.00 62.11 O
HETATM 2323  O   HOH    87      29.601  58.691 -24.045  1.00 49.94 O
HETATM 2324  O   HOH    88      22.701  60.581  -7.832  1.00 65.08 O
HETATM 2325  O   HOH    89      21.940  62.739 -12.104  1.00 60.23 O
HETATM 2326  O   HOH    90      28.142  44.638 -19.542  1.00 52.86 O
HETATM 2327  O   HOH    91      19.926  59.567 -10.713  1.00 54.05 O
HETATM 2328  O   HOH    92      23.841  23.097  24.364  1.00 55.20 O
HETATM 2329  O   HOH    93      14.026  37.104  24.024  1.00 50.35 O
HETATM 2330  O   HOH    94      28.637  30.316  16.747  1.00 47.63 O
HETATM 2331  O   HOH    95      13.597 -12.079  32.292  1.00 47.38 O
HETATM 2332  O   HOH    96      20.525   6.030  31.726  1.00 59.12 O
HETATM 2333  O   HOH    97      12.219  25.294  38.142  1.00 74.46 O
HETATM 2334  O   HOH    98      17.582  46.166 -21.327  1.00 58.26 O
HETATM 2335  O   HOH    99      18.462   3.098  17.614  1.00 74.29 O
HETATM 2336  O   HOH   100       7.657  -6.217  21.068  1.00 54.31 O
HETATM 2337  O   HOH   101      31.973  58.468 -22.566  1.00 51.37 O
HETATM 2338  O   HOH   102      25.581  34.891  15.303  1.00 62.92 O
HETATM 2339  O   HOH   103       9.781   4.793  26.865  1.00 52.97 O
HETATM 2340  O   HOH   104      27.113  28.768  14.346  1.00 46.27 O
HETATM 2341  O   HOH   105      20.934  59.591  -4.081  1.00 63.10 O
HETATM 2342  O   HOH   106      29.101  39.039  -6.576  1.00 50.94 O
HETATM 2343  O   HOH   107      20.829  -6.266  36.888  1.00 67.77 O
HETATM 2344  O   HOH   108      14.801  -6.395  38.213  1.00 57.81 O
HETATM 2345  O   HOH   109      21.412 -19.178  24.173  1.00 57.65 O
HETATM 2346  O   HOH   110      29.742  32.206  15.564  1.00 51.50 O
HETATM 2347  O   HOH   111      27.197  38.482  -3.772  1.00 57.43 O
HETATM 2348  O   HOH   112      23.730  20.567  24.733  1.00 63.78 O
HETATM 2349  O   HOH   113      15.996  50.339  -4.519  1.00 68.59 O
HETATM 2350  O   HOH   114      10.665  -4.867  34.503  1.00 53.34 O
HETATM 2351  O   HOH   115       6.955  17.535  26.540  1.00 72.17 O
HETATM 2352  O   HOH   116      15.712 -29.078  24.014  1.00 65.77 O
HETATM 2353  O   HOH   118      32.255  44.366  -7.537  1.00 62.15 O
HETATM 2354  O   HOH   119      29.827  41.068  -0.664  1.00 57.67 O
HETATM 2355  O   HOH   122      14.630 -27.859  26.706  1.00 65.41 O
HETATM 2356  O   HOH   123       8.521 -18.764  25.803  1.00 74.48 O
HETATM 2357  O   HOH   125      15.199  60.049 -12.759  1.00 63.41 O
HETATM 2358  O   HOH   126      10.378  14.473  18.707  1.00 52.05 O
HETATM 2359  O   HOH   127      28.187 -10.553  30.862  1.00 65.81 O
HETATM 2360  O   HOH   128       7.837  37.705   8.662  1.00 62.54 O
HETATM 2361  O   HOH   130      23.744  37.155   1.565  1.00 65.13 O
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Figure 2 (Table 2 (page 50))

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HETATM 2362  O   HOH   131      13.354  57.052  -9.380  1.00 64.16 O
HETATM 2363  O   HOH   132      31.235  44.417 -16.467  1.00 58.09 O
HETATM 2364  O   HOH   134      18.966  44.757   7.268  1.00 51.54 O
HETATM 2365  O   HOH   135      22.888   3.287  35.759  1.00 66.29 O
HETATM 2366  O   HOH   136      10.345  29.244  10.371  1.00 53.80 O
HETATM 2367  O   HOH   137      21.314  -8.331  20.298  1.00 59.91 O
HETATM 2368  O   HOH   138      38.747  55.169 -17.210  1.00 61.68 O
HETATM 2369  O   HOH   139      14.760  55.271  10.174  1.00 55.52 O
HETATM 2370  O   HOH   140      23.711  55.591   3.512  1.00 78.73 O
HETATM 2371  O   HOH   142       5.285  37.922   7.977  1.00 63.10 O
HETATM 2372  O   HOH   143      24.355  15.578  30.186  1.00 68.63 O
HETATM 2373  O   HOH   144      23.201   9.987  31.463  1.00 64.84 O
HETATM 2374  O   HOH   145      15.111  -8.434  40.304  1.00 70.85 O
HETATM 2375  O   HOH   146      34.105  49.705  -9.362  1.00 66.43 O
HETATM 2376  O   HOH   147      22.545  50.730   2.853  1.00 70.28 O
HETATM 2377  O   HOH   149      23.888  38.804 -17.868  1.00 69.84 O
HETATM 2378  O   HOH   150      26.301  66.907 -32.270  1.00 69.82 O
HETATM 2379  O   HOH   151      29.578  51.924 -24.078  1.00 67.26 O
HETATM 2380  O   HOH   152      31.935  49.759  -6.982  1.00 72.11 O
HETATM 2381  O   HOH   153      11.771  12.964  31.927  1.00 70.57 O
HETATM 2382  O   HOH   154      14.696   6.619  31.148  1.00 64.86 O
HETATM 2383  O   HOH   155      33.398  69.714 -31.980  1.00 74.81 O
HETATM 2384  O   HOH   156      26.480  50.982   0.230  1.00 59.10 O
HETATM 2385  O   HOH   157      22.798   7.195  30.848  1.00 68.26 O
HETATM 2386  O   HOH   158      19.477  -6.906  18.703  1.00 72.82 O
HETATM 2387  O   HOH   159      13.208  60.522 -15.082  1.00 57.68 O
HETATM 2388  O   HOH   160      34.799  47.949 -14.048  1.00 71.55 O
HETATM 2389  O   HOH   161      12.156 -20.278  36.293  1.00 63.41 O
HETATM 2390  O   HOH   162      12.064   0.618  21.733  1.00 59.67 O
HETATM 2391  O   HOH   163      13.025  12.470  18.298  1.00 57.94 O
HETATM 2392  O   HOH   164      11.241  -6.036  37.279  1.00 66.37 O
HETATM 2393  O   HOH   165      15.326  30.761   7.083  1.00 72.54 O
HETATM 2394  O   HOH   166      24.166  26.288   8.146  1.00 80.46 O
HETATM 2395  O   HOH   167      18.532  37.307  28.877  1.00 52.52 O
HETATM 2396  O   HOH   169      19.929  10.591  15.027  1.00 79.89 O
HETATM 2397  O   HOH   171      18.161  19.995  12.208  1.00 88.12 O
HETATM 2398  O   HOH   172      25.181 -23.987  37.247  1.00 83.59 O
HETATM 2399  O   HOH   174      18.136  -3.696  37.260  1.00 58.69 O
HETATM 2400  O   HOH   175       9.790  35.898   8.924  1.00 68.04 O
HETATM 2401  O   HOH   176      39.649  55.783 -13.588  1.00 75.74 O
HETATM 2402  O   HOH   177      11.431 -13.326  32.112  1.00 68.92 O
HETATM 2403  O   HOH   178      15.462  13.080  15.436  1.00 72.04 O
HETATM 2404  O   HOH   179      10.845 -23.387  30.834  1.00 75.68 O
HETATM 2405  O   HOH   180       8.771  -8.704  37.430  1.00 69.36 O
HETATM 2406  O   HOH   181      21.236  41.306 -18.704  1.00 71.93 O
HETATM 2407  O   HOH   182      15.632  39.325  24.779  1.00 76.42 O
HETATM 2408  O   HOH   184       9.633   7.268  24.170  1.00 59.85 O
HETATM 2409  O   HOH   185       8.212  -4.659  26.095  1.00 73.13 O
HETATM 2410  O   HOH   187      22.544 -23.667  22.886  1.00 67.43 O
HETATM 2411  O   HOH   190      38.135  52.923 -18.866  1.00 60.86 O
HETATM 2412  O   HOH   192      13.987 -13.566  39.379  1.00 64.17 O
HETATM 2413  O   HOH   194       8.678  19.753  34.818  1.00 74.26 O
HETATM 2414  O   HOH   195      16.248  11.313  17.210  1.00 71.99 O
HETATM 2415  O   HOH   196      21.583  37.449 -18.466  1.00 74.25 O
HETATM 2416  O   HOH   197      18.608  13.183  13.886  1.00 69.55 O
HETATM 2417  O   HOH   199      32.100  47.030 -11.918  1.00 55.13 O
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Figure 2 (Table 2 (page 51))

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HETATM 2418  O   HOH   200       8.309  -2.904  23.865  1.00 78.50 O
HETATM 2419  O   HOH   201      27.690  42.102   3.955  1.00 77.78 O
HETATM 2420  O   HOH   204      13.069  56.872  -6.846  1.00 79.77 O
HETATM 2421  O   HOH   205      13.299   3.871  18.787  1.00 66.67 O
HETATM 2422  O   HOH   206      29.245  60.023 -30.224  1.00 60.72 O
HETATM 2423  O   HOH   208      14.879  -4.423  17.190  1.00 90.36 O
HETATM 2424  O   HOH   209      10.483  17.298  32.627  1.00 73.09 O
HETATM 2425  O   HOH   210      11.855  61.308 -30.434  1.00 88.84 O
HETATM 2426  O   HOH   211      13.217  40.439  25.017  1.00 85.86 O
HETATM 2427  O   HOH   213       7.822 -16.528  22.942  1.00 78.51 O
HETATM 2428  O   HOH   214      23.675  20.955  33.560  1.00 73.68 O
HETATM 2429  O   HOH   215       8.958 -13.070  31.871  1.00 66.49 O
HETATM 2430  O   HOH   216      13.965   9.052  16.630  1.00 67.53 O
HETATM 2431  O   HOH   220       8.596  -0.069  28.112  1.00 61.80 O
HETATM 2432  O   HOH   221      31.299  38.557 -18.341  1.00 61.93 O
HETATM 2433  O   HOH   222      20.516  15.336  17.249  1.00 62.41 O
HETATM 2434  O   HOH   223      32.487  45.347 -13.991  1.00 67.08 O
HETATM 2435  O   HOH   224       9.634  26.343  28.605  1.00 80.33 O
HETATM 2436  O   HOH   225      26.881  41.843   6.770  1.00 66.49 O
HETATM 2437  O   HOH   226      21.933  62.656  -9.449  1.00 77.20 O
HETATM 2438  O   HOH   227      16.939  -0.959  38.266  1.00 47.64 O
HETATM 2439  O   HOH   228       1.517  27.871  29.550  1.00 69.94 O
HETATM 2440  O   HOH   229      25.455  67.088 -17.467  1.00 70.28 O
HETATM 2441  O   HOH   231      22.761  36.354 -14.024  1.00 67.12 O
HETATM 2442  O   HOH   233       9.742 -18.263  29.864  1.00 71.11 O
HETATM 2443  O   HOH   236       9.749  -1.644  39.210  1.00 68.73 O
HETATM 2444  O   HOH   238      18.795  37.370  -0.374  1.00 70.06 O
HETATM 2445  O   HOH   239      28.893 -23.822  27.314  1.00 63.21 O
HETATM 2446  O   HOH   240      20.653  54.689  -2.794  1.00 69.17 O
HETATM 2447  O   HOH   241      32.703  57.255  -7.932  1.00 73.68 O
HETATM 2448  O   HOH   242      26.839  45.754 -28.862  1.00 73.66 O
HETATM 2449  O   HOH   243      21.145  36.229  -1.718  1.00 67.47 O
HETATM 2450  O   HOH   244      24.749  63.978 -31.459  1.00 70.06 O
HETATM 2451  O   HOH   245      15.031  42.223  -0.424  1.00 65.72 O
HETATM 2452  O   HOH   246      13.421  46.493   5.518  1.00 68.84 O
HETATM 2453  O   HOH   247      31.086  37.829 -20.633  1.00 67.16 O
HETATM 2454  O   HOH   249      16.331  24.733   8.656  1.00 80.75 O
HETATM 2455  O   HOH   250      34.686  48.482 -11.577  1.00 67.41 O
HETATM 2456  O   HOH   252      26.863 -21.667  27.711  1.00 73.87 O
HETATM 2457  O   HOH   253      25.486  24.675   5.799  1.00 94.36 O
HETATM 2458  O   HOH   255      19.570 -18.069  15.539  1.00 68.87 O
HETATM 2459  O   HOH   256       7.507  24.181  27.128  1.00 75.95 O
HETATM 2460  O   HOH   257      18.214  50.275  13.595  1.00 77.43 O
HETATM 2461  O   HOH   258      24.259   5.598  21.754  1.00 80.04 O
HETATM 2462  O   HOH   259      23.644  -9.401  38.458  1.00 73.87 O
HETATM 2463  O   HOH   260      29.288  57.908 -36.191  1.00 83.70 O
HETATM 2464  O   HOH   261      14.644 -13.020  15.667  1.00 67.62 O
HETATM 2465  O   HOH   262      16.016  47.827  16.745  1.00 77.21 O
HETATM 2466  O   HOH   263      19.538 -33.347  29.648  1.00 64.40 O
HETATM 2467  O   HOH   265       2.949  33.426  13.572  1.00 75.54 O
HETATM 2468  O   HOH   266      25.030  51.698 -23.955  1.00 72.53 O
HETATM 2469  O   HOH   267      29.126  34.667  -5.967  1.00 87.07 O
HETATM 2470  O   HOH   268      21.351   0.866  18.679  1.00 81.24 O
HETATM 2471  O   HOH   270      11.563 -28.282  33.256  1.00 88.99 O
HETATM 2472  O   HOH   273      25.953  36.560 -14.131  1.00 68.45 O
HETATM 2473  O   HOH   275       3.498  32.668  11.344  1.00 60.17 O
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Figure 2 (Table 2 (page 52))

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HETATM 2474  O   HOH   277      24.261 -20.185  20.738  1.00 69.47 O
HETATM 2475  O   HOH   279      16.935  12.111  32.241  1.00 61.50 O
HETATM 2476  O   HOH   281       6.985  31.018  33.495  1.00 82.04 O
HETATM 2477  O   HOH   282      29.259  66.155 -18.386  1.00 76.82 O
HETATM 2478  O   HOH   283       7.960  15.959  16.209  1.00 82.31 O
HETATM 2479  O   HOH   284      10.497 -27.436  17.219  1.00 87.04 O
HETATM 2480  O   HOH   286      26.964  63.396 -39.492  1.00 92.90 O
HETATM 2481  O   HOH   288      24.134  68.136 -30.170  1.00 73.68 O
HETATM 2482  O   HOH   289      21.035  57.596  -2.427  1.00 63.71 O
HETATM 2483  O   HOH   290       5.098  -6.663   9.498  1.00 71.30 O
HETATM 2484  O   HOH   291      28.355  60.022 -32.628  1.00 84.14 O
HETATM 2485  O   HOH   292      27.829 -18.993  32.106  1.00 83.61 O
HETATM 2486  O   HOH   294      25.765  53.781 -27.581  1.00 80.50 O
HETATM 2487  O   HOH   295      24.969 -15.013  17.181  1.00 79.45 O
HETATM 2488  O   HOH   296      21.804 -31.840  29.638  1.00 63.37 O
HETATM 2489  O   HOH   297      24.675  41.475  22.470  1.00 76.81 O
HETATM 2490  O   HOH   298      21.097 -16.469  16.858  1.00 76.40 O
HETATM 2491  O   HOH   299      10.492   1.947  39.785  1.00 73.55 O
HETATM 2492  O   HOH   300      24.883  60.577  -6.394  1.00 83.17 O
HETATM 2493  O   HOH   301      12.022  63.003 -25.379  1.00 82.86 O
HETATM 2494  O   HOH   302      29.658  36.500 -13.658  1.00 76.81 O
HETATM 2495  O   HOH   303      28.183  35.860 -10.762  1.00 71.74 O
HETATM 2496  O   HOH   304      33.215  39.854  -9.262  1.00 79.17 O
HETATM 2497  O   HOH   305      22.138  35.777 -10.127  1.00 75.26 O
HETATM 2498  O   HOH   306      34.862  51.476  -6.285  1.00 73.10 O
HETATM 2499  O   HOH   307      40.147  51.580  -7.567  1.00 79.78 O
HETATM 2500  O   HOH   308      28.423  71.917 -29.800  1.00 75.06 O
HETATM 2501  O   HOH   309      31.298  68.573 -22.781  1.00 78.92 O
HETATM 2502  O   HOH   310      22.252  33.788   4.586  1.00 75.58 O
HETATM 2503  O   HOH   311      26.312  13.773  26.214  1.00 71.75 O
HETATM 2504  O   HOH   312      24.723  12.029  25.114  1.00 75.67 O
HETATM 2505  O   HOH   313      23.485  49.266   5.646  1.00 72.55 O
HETATM 2506  O   HOH   314      25.648  43.055  12.920  1.00 71.36 O
HETATM 2507  O   HOH   315       4.653  34.503  32.710  1.00 77.71 O
HETATM 2508  O   HOH   316       2.456  37.131  32.175  1.00 78.77 O
HETATM 2509  O   HOH   317       6.881  27.100  34.488  1.00 80.24 O
HETATM 2510  O   HOH   318      10.082  23.711  13.099  1.00 81.07 O
HETATM 2511  O   HOH   319      18.524 -28.499  21.428  1.00 79.53 O
HETATM 2512  O   HOH   321      26.684   3.017  30.716  1.00 82.34 O
HETATM 2513  O   HOH   322      27.178  -5.228  32.903  1.00 82.07 O
CONECT  174  603
CONECT  603  174
CONECT  932 1341
CONECT 1341  932
CONECT 1686 2094
CONECT 2094 1686
MASTER      303    0    0    3   27    0    0    6 2512    1    6 23
END
```

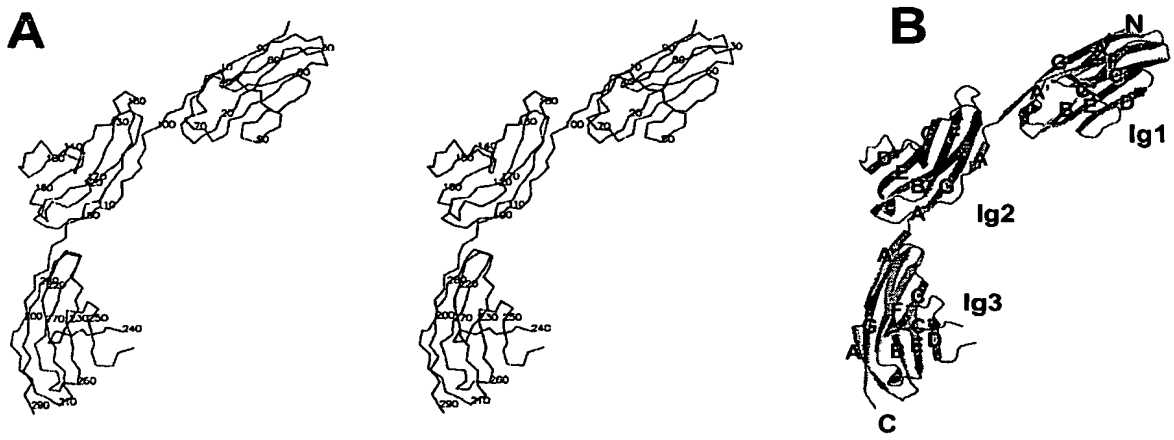


Figure 3

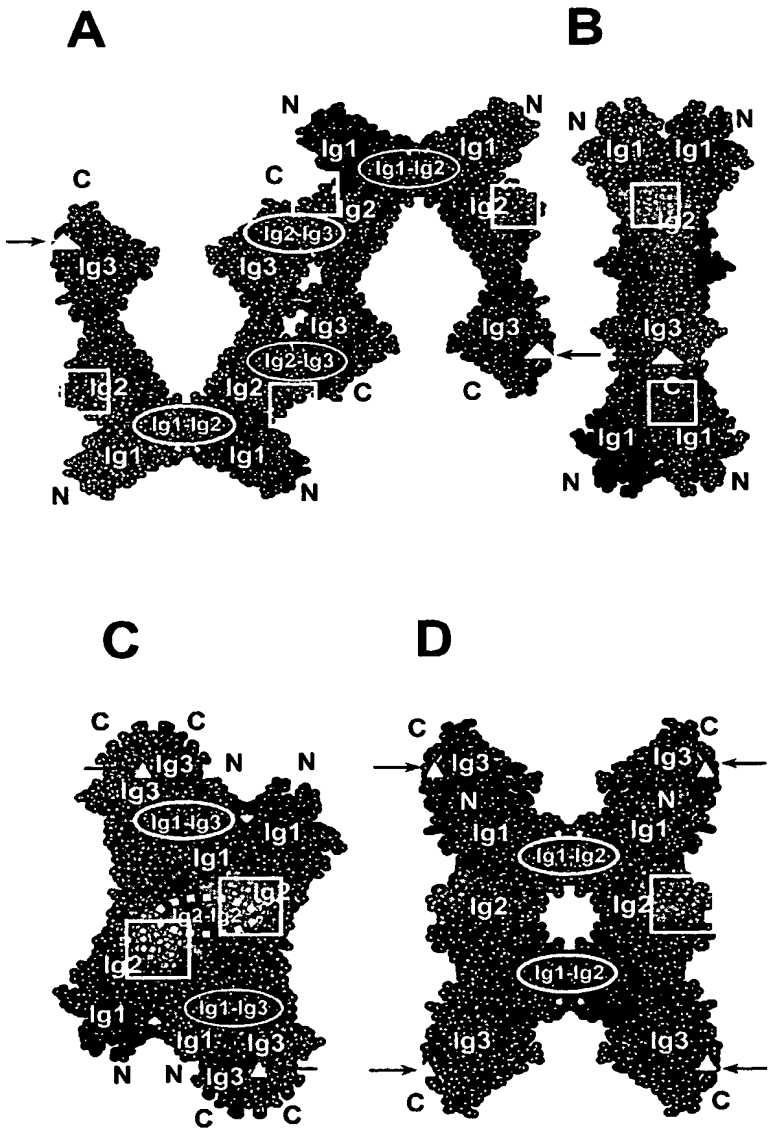


Figure 4

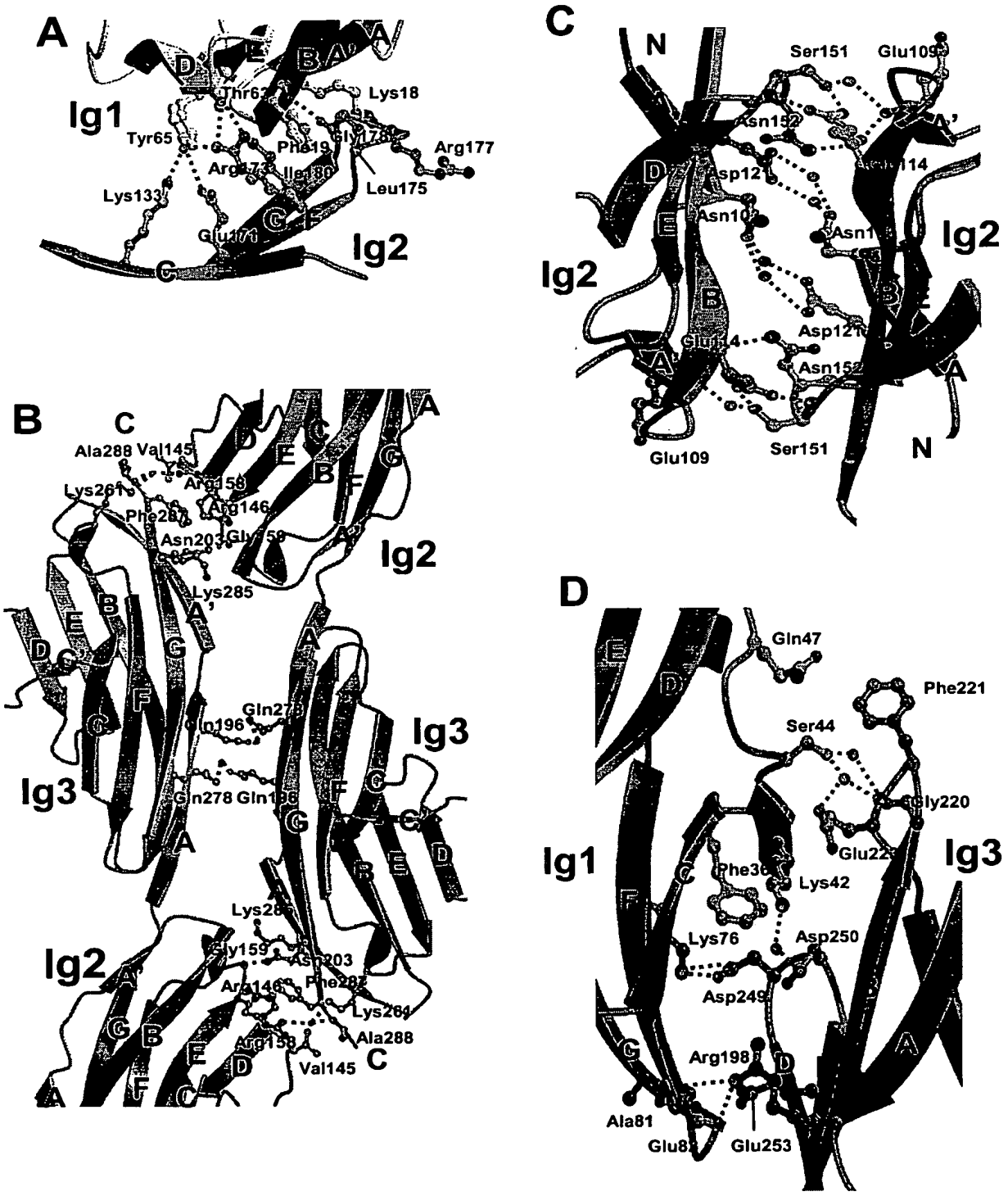
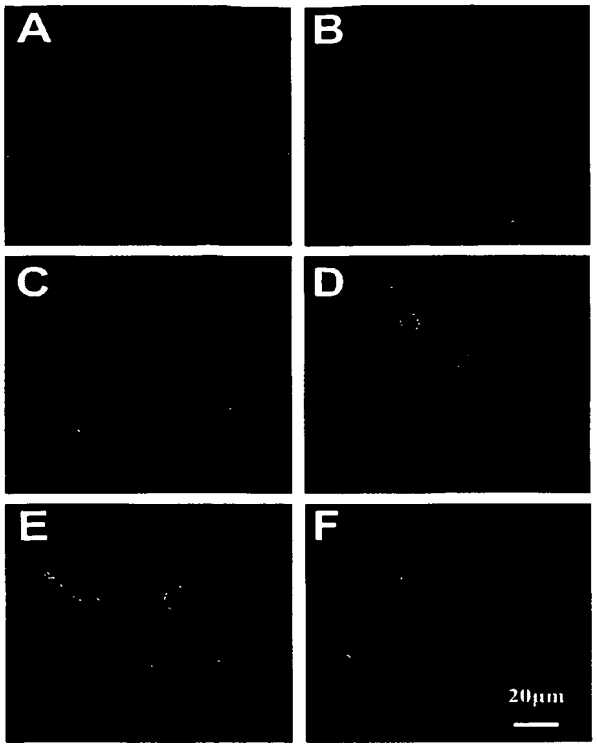

A
Ig1
Ig2
Lys18
Tyr65
Phe19
Arg177
Leu175
Lys133
Glu171
B
C
Ala288
Val145
Arg158
Lys261
Arg146
Phe287
Asn203
Lys285
Ig2
Ig3
Gln278
Gln196
Lys284
Gly159
Asn203
Arg146
Phe287
Lys264
Ala288
Arg158
Val145
C
N
Ser151
Glu109
Asn152
Asp121
Asn102
Ig2
Glu114
Asp121
Asn152
Glu109
Ser151
N
D
Gln47
Phe221
Ser44
Gly220
Glu223
Ig1
Ig3
Phe36
Lys42
Lys76
Asp250
Asp249
Arg198
Ala81
Glu82
Glu253

Figure 5


A
B
C
D
E
F
20µm

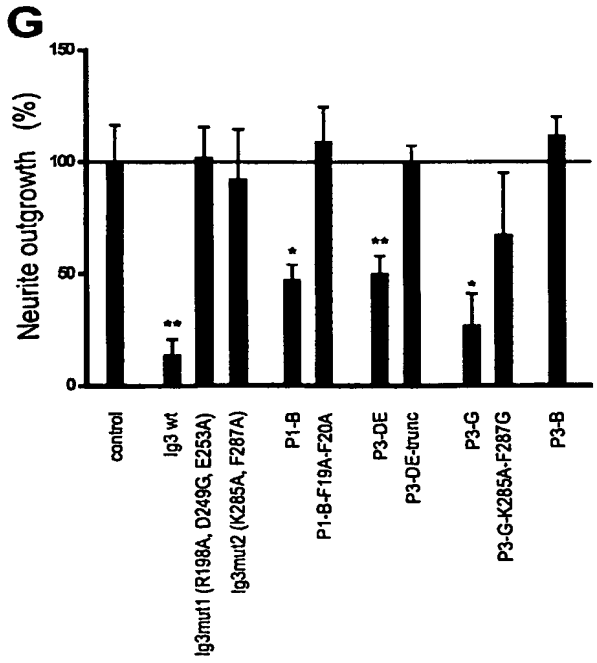

G
Neurite outgrowth (%)
150
100
50
0
control
Ig3 wt
Ig3mut1 (R198A, D249G, E253A)
Ig3mut2 (K285A, F287A)
P1-B
P1-B-F19A-F20A
P3-DE
P3-DE-trunc
P3-G
P3-G-K285A-F287G
P3-B

Figure 6

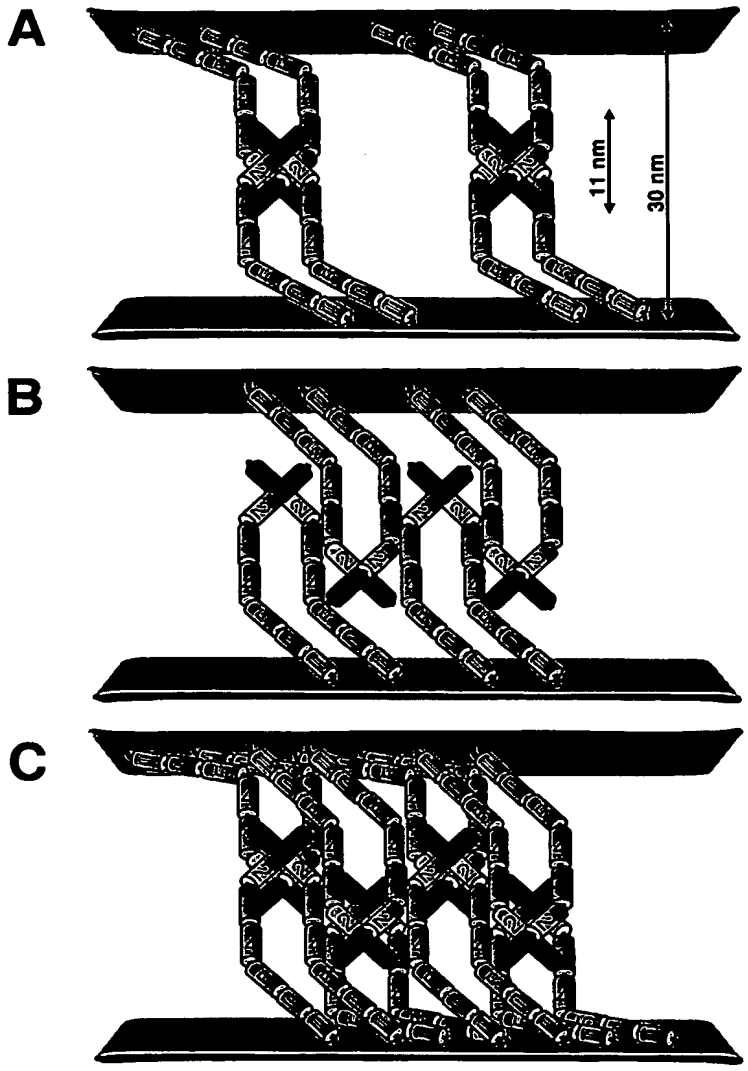


Figure 7

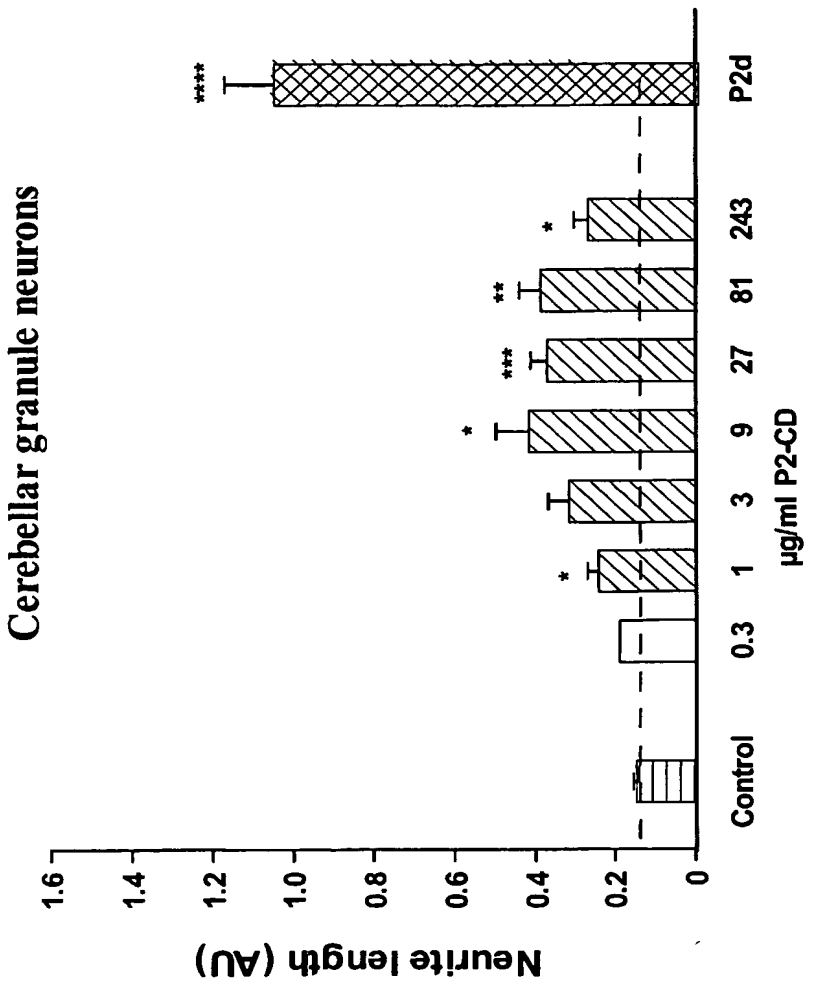

Cerebellar granule neurons
Neurite length (AU)
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
Control
0.3
1
3
9
27
81
243
P2d
µg/ml P2-CD
*
*
***
**
*
****

Figure 8

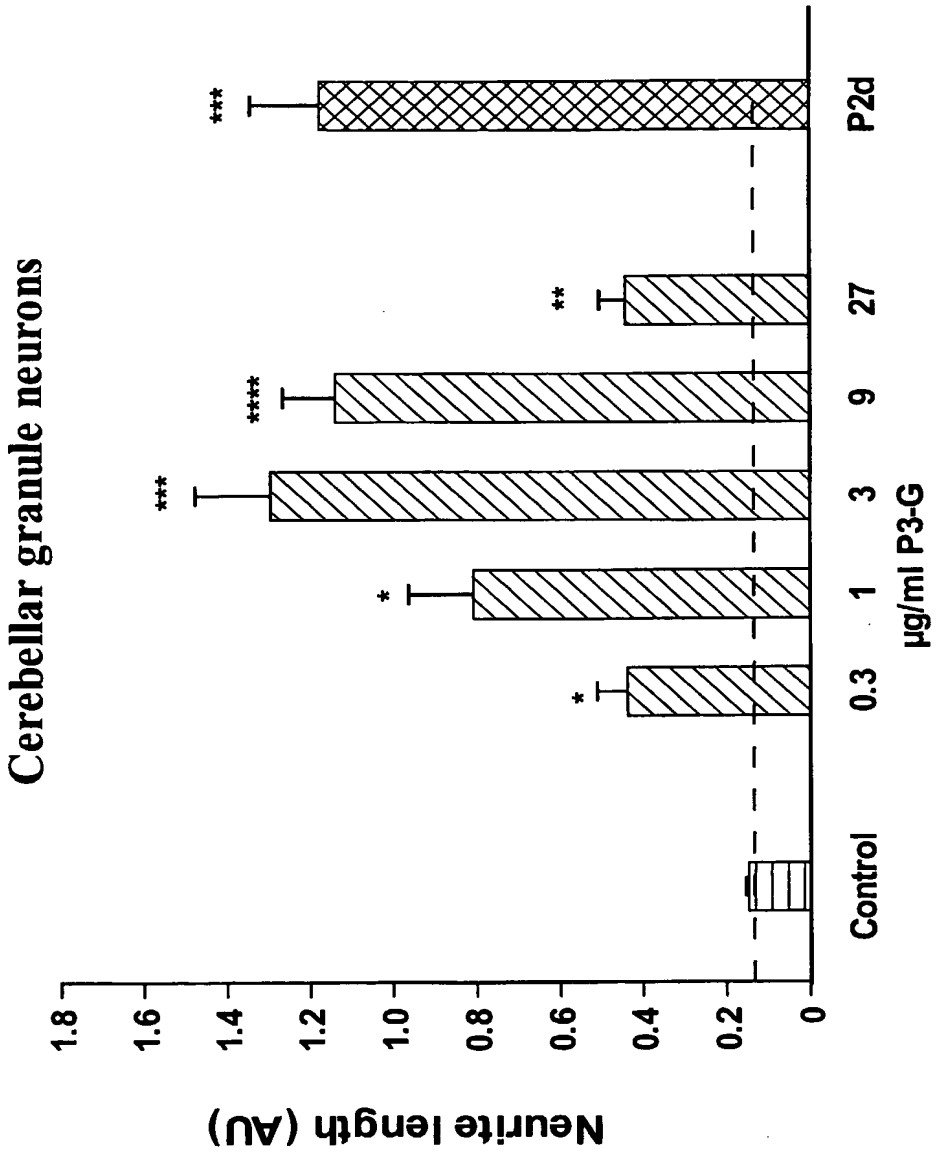

Cerebellar granule neurons
Neurite length (AU)
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
Control
0.3
1
3
9
27
P2d
µg/ml P3-G
*
*
***
****
**
***

Figure 9

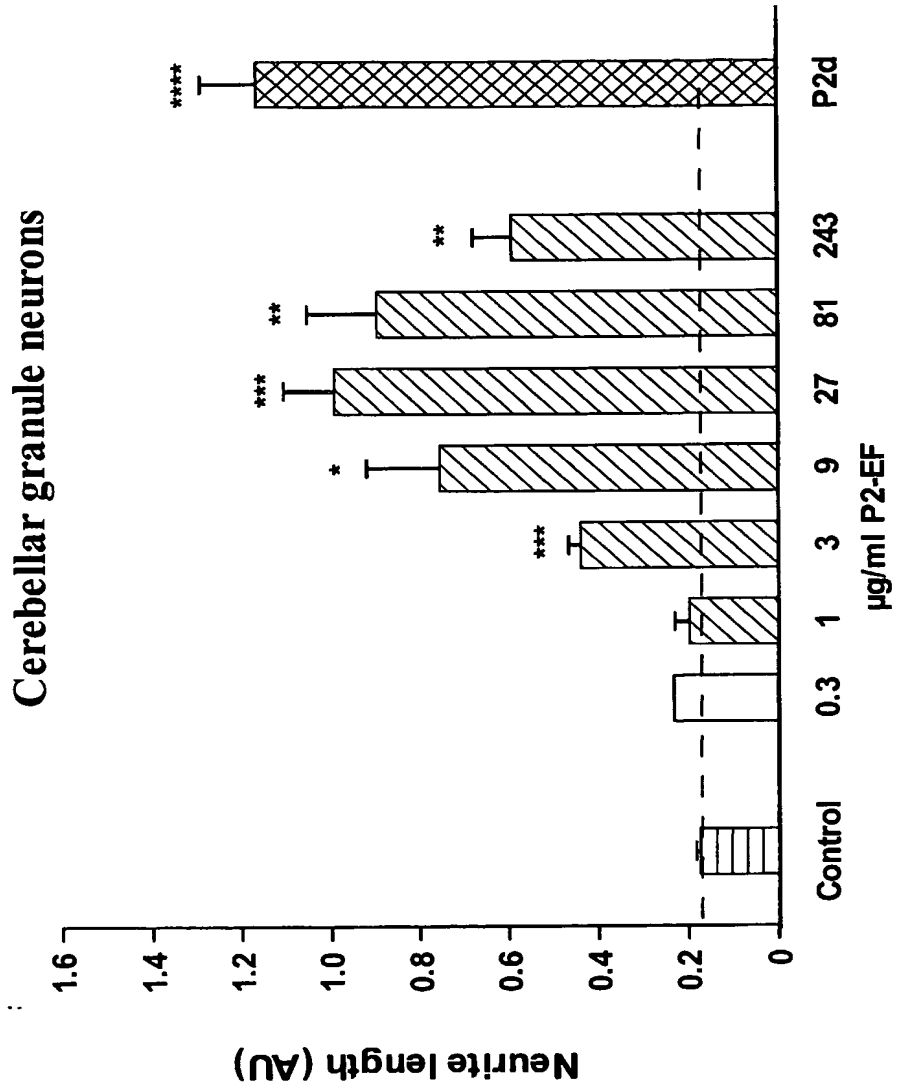

Cerebellar granule neurons
Neurite length (AU)
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
Control
0.3
1
3
9
27
81
243
P2d
µg/ml P2-EF
****
**
***
*
***
**
***

Figure 10

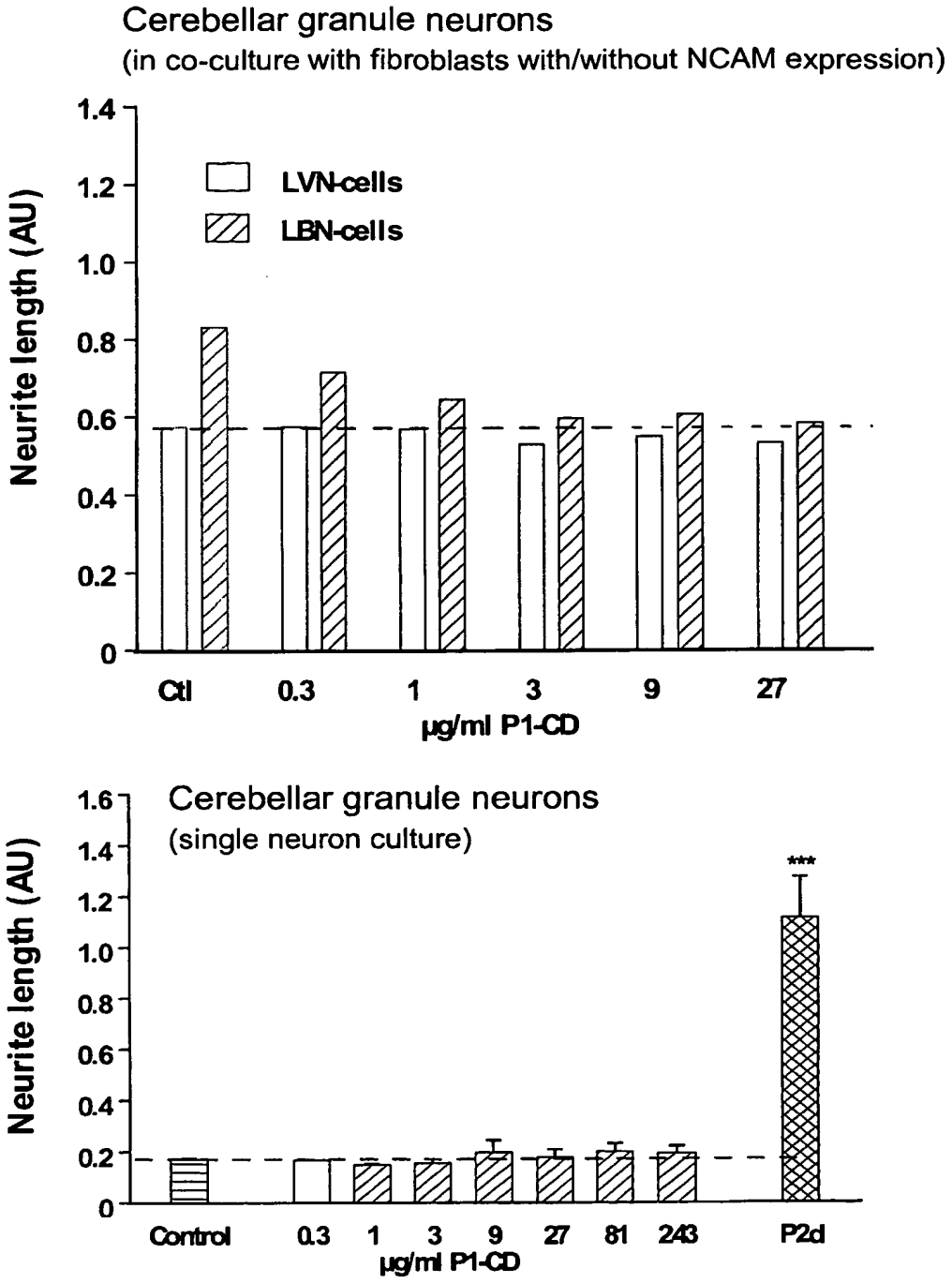

Cerebellar granule neurons
(in co-culture with fibroblasts with/without NCAM expression)
Neurite length (AU)
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
LVN-cells
LBN-cells
Ctl
0.3
1
3
9
27
µg/ml P1-CD
Cerebellar granule neurons
(single neuron culture)
Neurite length (AU)
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
***
Control
0.3
1
3
9
27
81
243
P2d
µg/ml P1-CD

Figure 11

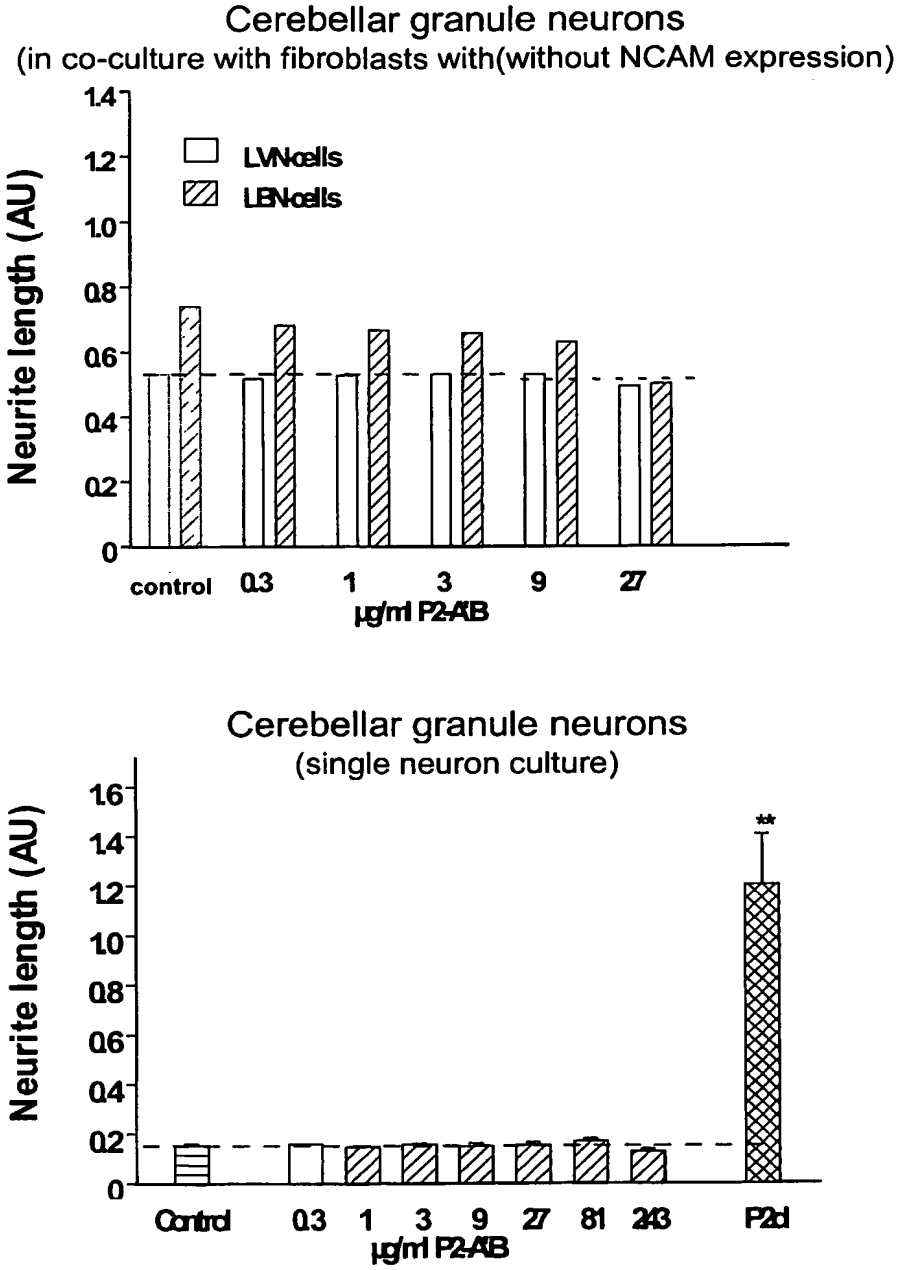

Cerebellar granule neurons
(in co-culture with fibroblasts with(without NCAM expression)
Neurite length (AU)
LVNcells
LBNcells
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
control
0.3
1
3
9
27
µg/ml P2-AB
Cerebellar granule neurons
(single neuron culture)
Neurite length (AU)
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
**
Control
0.3
1
3
9
27
81
243
P2cl
µg/ml P2-AB

Figure 12

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